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May 5, 2020

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Abstract

We introduce a numerical framework for dispersive equations embedding their underlying resonance structure into the discretisation. This will allow us to resolve the nonlinear oscillations of the PDE and to approximate with high order accuracy a large class of equations under lower regularity assumptions than classical techniques require. The key idea to control the nonlinear frequency interactions in the system up to arbitrary high order thereby lies in a tailored decorated tree formalism. Our algebraic structures are close to the ones developed for singular SPDEs with Regularity Structures. We adapt them to the context of dispersive PDEs by using a novel class of decorations which encode the dominant frequencies. The structure proposed in this paper is new and gives a variant of the Butcher-Connes-Kreimer Hopf algebra on decorated trees. We observe a similar Birkhoff type factorisation as in SPDEs and perturbative quantum field theory. This factorisation allows us to single out oscillations and to optimise the local error by mapping it to the particular regularity of the solution. The field of singular SPDEs took advantage of numerical methods and renormalisation in perturbative quantum field theory by extending their structures via the adjunction of decorations and Taylor expansions. Now, through this work, Numerical Analysis is taking advantage of these extended structures and provides a new perspective on them.

Contents

1 Introduction

We consider nonlinear dispersive equations

$$\begin{aligned} &i\partial_t u(t,x) + \mathscr{L}\left(\nabla, \frac{1}{\varepsilon}\right) u(t,x) = |\nabla|^\alpha p(u(t,x), \overline{u}(t,x)) \\ &u(0,x) = v(x) \end{aligned} \tag{1.1}$$

where we assume a polynomial nonlinearity p and that the structure of (1.1) implies at least local wellposedness of the problem on the finite time interval $]0,T]$, $T<\infty$. Here, u is the complex-valued solution that we want to approximate.

In the last decades, Strichartz estimates and Bourgain spaces allowed to establish well-posedness results for dispersive equations in low regularity spaces [9, 15, 56, 71, 72]. Numerical theory for dispersive PDEs, on the other hand, is in general still restricted to smooth solutions. This is due to the fact that most classical approximation techniques were originally developed for linear problems and thus, in general, neglect nonlinear frequency interactions in a system. In the dispersive setting (1.1) the interaction of the differential operator $\mathscr{L}$ with the nonlinearity p triggers oscillations both in space and in time and, unlike for parabolic problems, no smoothing can be expected. At low regularity and high oscillations, these nonlinear frequency interactions play an essential role: Note that while the influence of $i\mathscr{L}$ can be small, the influence of the interaction of $+i\mathscr{L}$ and $-i\mathscr{L}$ can be huge, and vice versa. Classical *linearised* frequency approximations, as e.g., in Table 1 below, are therefore restricted to smooth solutions. The latter is not only a technical formality: The severe order reduction in case of non-smooth solutions is also observed numerically, see, e.g., [54, 67] and Figure 2, and only little is known on how to overcome this. For an extensive overview on numerical methods for Hamiltonian systems, geometric numerical analysis, structure preserving algorithms, and highly oscillatory problems we refer to the books Butcher [17], Engquist et al. [34], Faou [35], E. Hairer et al. [42, 43], Holden et al. [48], Leimkuhler &

Reich [59], McLachlan & Quispel [63], Sanz-Serna & Calvo [69] and the references therein.

In this work, we establish a new framework of resonance based approximations for dispersive equations which will allow us to solve with high order accuracy a large class of equations under (much) lower regularity assumptions than classical techniques require. The key in the construction of the new methods lies in analysing the underlying oscillatory structure of the system (1.1). We look at the corresponding mild solution given by Duhamel's formula

$$u(t) = e^{it\mathscr{L}(\nabla,\frac{1}{\varepsilon})}v - ie^{it\mathscr{L}(\nabla,\frac{1}{\varepsilon})}|\nabla|^{\alpha}\int_0^t e^{-i\xi\mathscr{L}(\nabla,\frac{1}{\varepsilon})}p(u(\xi),\overline{u}(\xi))d\xi \tag{1.2}$$

and its iterations

$$u(t) = e^{it\mathscr{L}(\nabla,\frac{1}{\varepsilon})}v - ie^{it\mathscr{L}(\nabla,\frac{1}{\varepsilon})}|\nabla|^{\alpha}\mathscr{I}_1(t,\mathscr{L},v,p) + |\nabla|^{2\alpha}\int_0^t\int_0^{\xi}\ldots d\xi_1 d\xi. \tag{1.3}$$

The principal oscillatory integral thereby takes the form

$$\mathscr{I}_1(t,\mathscr{L},v,p) = \int_0^t \mathcal{O}\mathfrak{z}\mathfrak{c}(\xi,\mathscr{L},v,p)d\xi$$

with the central oscillations $\mathcal{O}\mathfrak{z}\mathfrak{c}$ driven by the nonlinear frequency interactions between the differential operator $\mathscr{L}$ and the nonlinearity p

$$\mathcal{O}\mathfrak{z}\mathfrak{c}(\xi,\mathscr{L},v,p) = e^{-i\xi\mathscr{L}(\nabla,\frac{1}{\varepsilon})}p\Big(e^{i\xi\mathscr{L}(\nabla,\frac{1}{\varepsilon})}v, e^{-i\xi\mathscr{L}(\nabla,\frac{1}{\varepsilon})}\overline{v}\Big). \tag{1.4}$$

In order to obtain a suitable approximation at low regularity, it is central to resolve these oscillations – characterised by the underlying structure of resonances – numerically. Classical linearised frequency approximations, however, neglect the nonlinear interactions in (1.4). This is also illustrated in Table 1 below for splitting and exponential methods ([43, 46]).

Numerical scheme	*Approximation on frequency level*
exponential method	$\mathcal{O}\mathfrak{z}\mathfrak{c}(\xi,\mathscr{L},v,p) \approx e^{-i\xi\mathscr{L}(\nabla,\frac{1}{\varepsilon})}p(v,\overline{v})$
splitting method	$\mathcal{O}\mathfrak{z}\mathfrak{c}(\xi,\mathscr{L},v,p) \approx p(v,\overline{v})$

Table 1: Classical frequency approximations of the principal oscillations (1.4).

The aim of this paper is to introduce a framework embedding the underlying nonlinear oscillations (1.4) of the PDE into the numerical discretisation. The main idea for tackling this problem is to use decorated trees which allow us to optimise the structure of the local error by mapping it to the particular regularity of the solution.

While first-order resonance-based discretisations have been presented for particular examples, e.g., the Nonlinear Schrödinger (NLS), Korteweg–de Vries (KdV), Boussinesq, Dirac and Klein–Gordon equation, see [4, 5, 47, 66, 67, 70], no general framework could be established so far. Each and every equation had to be targeted carefully one at a time based on a sophisticated resonance analysis. This is due to the fact that the structure of the underlying oscillations (1.4) strongly depends on the form of the leading operator $\mathscr{L}$, the nonlinearity p and in particular their nonlinear interaction.

In addition, to the lack of a general framework, only very little is known about the higher-order counterpart of resonance based discretisations. Indeed, some attempts have been made for second-order methods (see, e.g., [47] for KdV and [57] for NLS) but they are not optimal. This is due to the fact that the leading differential operator $\mathscr{L}$ triggers a full spectrum of frequencies $k_j \in \mathbf{Z}^d$ and up to now it was an unresolved issue on how to control their nonlinear interactions up to higher order.

To overcome this we introduce a new tailored decorated tree formalism. Thereby the decorated trees encode the Fourier coefficients in the iteration of Duhamel's formula, where the node decoration encodes the frequencies which is in the spirit close to [27, 41, 38]. The main difficulty then lies in controlling the nonlinear frequency interactions within these iterated integrals up to the desired order with the constraint of a given a priori regularity of the solution. The latter is achieved by embedding the underlying oscillations, and their higher order iterations, via well-chosen Taylor series expansions into our formalism: the dominant interactions will be integrated exactly whereas only the lower order parts are approximated within the discretisation.

We base our algebraic structures on the ones developed for SPDEs with Regularity Structure [44] which is a generalisation of Rough Paths [60, 61, 39, 40]. Part of the formalism is inspired by [12] and the recentering map used for giving a local description of the solution of a singular SPDEs. We adapt it to the context of dispersive PDEs by using a new class of decorated trees encoding the underlying dominant frequencies. The structure proposed in this paper is new and gives a variant of the Butcher-Connes-Kreimer Hopf algebra [16, 30] on decorated trees. We observe a similar Birkhoff type factorisation as in SPDEs and perturbative quantum field theory. This factorisation allows us to single out oscillations and to perform the local error analysis.

The framework of decorated trees and the underlying Hopf algebras have allowed the resolution of a large class of singular SPDEs [44, 12, 22, 11] which include a natural random dynamic on the space of loops in a Riemannian manifold in [14], see [13] for a very brief survey on these developments. With this general framework, one can study properties of singular SPDEs solutions in full subcritical-regimes [23, 6, 45, 24]. The formalism of decorated trees together with the description of the renormalised equation in this context (see [11]) was directly inspired from numerical analysis of ODEs, more precisely, from the characterisation of Runge-Kutta methods via B-series. Indeed, B-series are numerical (multi-)step methods for ODEs represented by a tree expansion, see, e.g., [16, 7, 26, 43, 53, 19]. We also

refer to [64] for a review of B-series on Lie groups and homogeneous manifolds as well as to [65] providing an alternative structure via word series. The field of singular SPDEs took advantage of the B-series formalism and extended their structures via the adjunction of decorations and Taylor expansions. Now, through this work, Numerical Analysis is taking advantage of these extended structures and enlarges their scope.

Assumptions. We impose periodic boundary condition that is $x \in \mathbf{T}^d$. However, our theory can be extended to the full space $\mathbf{R}^d$. We assume that the differential operator $\mathscr{L}$ is real and consider two types of structures of the system (1.1).

- The differential operators $\mathscr{L}\big(\nabla, \frac{1}{\varepsilon}\big) = \mathscr{L}(\nabla)$ and $|\nabla|^\alpha$ cast in Fourier space into the form

$$\mathscr{L}(\nabla)(k) = k^\sigma + \prod_{\sum \gamma_j < \sigma} k_j^{\gamma_j}, \qquad |\nabla|^\alpha(k) = \prod_{\alpha = \sum \gamma_j < \sigma} k_j^{\gamma_j} \tag{1.6}$$

  where for $k = (k_1, \dots, k_d) \in \mathbf{Z}^d$ and $m = (m_1, \dots, m_d) \in \mathbf{Z}^d$ we set

$$k^\sigma = k_1^\sigma + \ldots + k_d^\sigma, \qquad k \cdot m = k_1 m_1 + \ldots + k_d m_d.$$

  This structure includes for instance the Schrödinger equation (Section A.1)

$$\mathscr{L}(\nabla) = \Delta, \qquad |\nabla|^\alpha = 1$$

  and the Korteweg–de Vries equation (Section A.2)

$$\mathscr{L}(\nabla) = i\partial_x^3, \qquad |\nabla|^\alpha = i\partial_x.$$

- We also consider the setting of a given finite set of high frequencies $\frac{1}{|\varepsilon_j|} \gg 1$, $1 \le j \le J$. In this case we assume that the operators $\mathscr{L}\big(\nabla, \frac{1}{\varepsilon}\big)$ and $|\nabla|^\alpha$ take the form

$$\mathscr{L}\left(\nabla, \frac{1}{\varepsilon}\right) = \prod_j \frac{1}{\varepsilon_j^{\sigma_j}} + \mathscr{B}\left(\nabla, \frac{1}{\varepsilon}\right), \qquad |\nabla|^\alpha = \mathscr{C}\left(\nabla, \frac{1}{\varepsilon}\right) \tag{1.7}$$

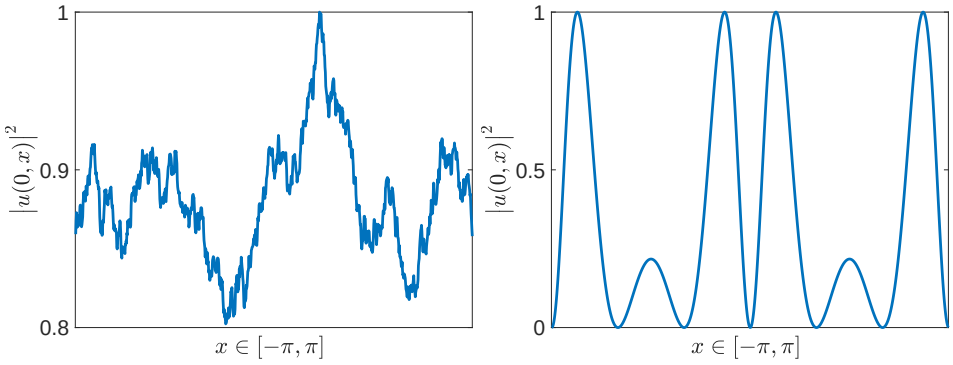
  for some differential operators $\mathscr{B}\big(\nabla, \frac{1}{\varepsilon}\big)$ and $\mathscr{C}\big(\nabla, \frac{1}{\varepsilon}\big)$ which can be bounded uniformly in $\min_j |\varepsilon_j|$ and are relatively bounded by differential operators of degree σ and degree $\alpha < \sigma$, respectively. This allows us to include highly oscillatory Klein–Gordon type equations (Section A.3).

In the next section we introduce our resonance based technique to solve the dispersive PDE (1.1).

1.1 Resonances as a computational tool

Instead of employing classical linearised frequency approximations as described in Table 1 we want to embed the underlying nonlinear resonance structure

$$\mathcal{O}\mathfrak{s}\mathfrak{c}(\xi, \mathscr{L}, v, p) = e^{-i\xi\mathscr{L}(\nabla, \frac{1}{\varepsilon})} p\Big(e^{i\xi\mathscr{L}(\nabla, \frac{1}{\varepsilon})} v, e^{-i\xi\mathscr{L}(\nabla, \frac{1}{\varepsilon})} \overline{v}\Big) \tag{1.8}$$



(a) H^1 data (b) $\mathscr{C}^\infty$ data

Figure 1: Initial values for Figure 2: $u_0 \in H^1$ (left) and $u_0 \in \mathscr{C}^\infty$ (right).

into the numerical discretisation. Ideally we would like to resolve all frequency interactions in (1.8). However, in general, these consequent into a generalised convolution (of Coifman–Meyer type [32]) which can not be converted as a product into the physical space. Thus the iteration would need to be carried out fully in Fourier space which does not yield a scheme which can be practically implemented in higher spatial dimensions, see also Remark 1.3 below.

In order to obtain an efficient and practical resonance based discretisation we extract the dominant and lower-order parts from the resonance structure (1.8). More precisely, we filter out the dominant parts $\mathscr{L}_{\text{dom}}$ and treat them exactly while only approximating the lower order terms in the spirit of

$$\mathfrak{Osc}(\xi, \mathscr{L}, v, p) = \Big[e^{i\xi\mathscr{L}_{\text{dom}}\left(\nabla, \frac{1}{\varepsilon}\right)} p_{\text{dom}}(v, \overline{v})\Big] p_{\text{low}}(v, \overline{v}) + \mathfrak{O}\Big(\xi \mathscr{L}_{\text{low}}(\nabla) v\Big). \quad (1.9)$$

Here, $\mathscr{L}_{\text{dom}}$ denotes a suitable dominant part of the high frequency interactions and

$$\mathscr{L}_{\text{low}} = \mathscr{L} - \mathscr{L}_{\text{dom}} \quad (1.10)$$

the corresponding non-oscillatory parts (details are given in Definition 2.5 below). The crucial issue is to determine $\mathscr{L}_{\text{dom}}$, p_{dom} and $\mathscr{L}_{\text{low}}, p_{\text{low}}$ in (1.9) with an interplay between keeping the underlying structure of PDE and allowing a practical implementation at a reasonable cost.

Thanks to the resonance based ansatz (1.9) the principal oscillatory integral

$$\mathscr{I}_1(t, \mathscr{L}, v, p) = \int_0^t \mathfrak{Osc}(\xi, \mathscr{L}, v, p) d\xi$$

in the expansion of the exact solution (1.3)

$$u(t) = e^{it\mathscr{L}\left(\nabla, \frac{1}{\varepsilon}\right)} v - i e^{it\mathscr{L}\left(\nabla, \frac{1}{\varepsilon}\right)} |\nabla|^\alpha \mathscr{I}_1(t, \mathscr{L}, v, p) + \mathfrak{O}\big(t^2 |\nabla|^{2\alpha} u\big) \quad (1.11)$$

then takes the form

$$\begin{aligned}\mathcal{I}_1(t,\mathscr{L},v,p) &= \int_0^t \Big[e^{i\xi\mathscr{L}_{\text{dom}}}p_{\text{dom}}(v,\overline{v})\Big]p_{\text{low}}(v,\overline{v}) + \mathcal{O}\Big(\xi\mathscr{L}_{\text{low}}(\nabla)v\Big)d\xi \\ &= tp_{\text{low}}(v,\overline{v})\varphi_1(it\mathscr{L}_{\text{dom}})p_{\text{dom}}(v,\overline{v}) + \mathcal{O}\Big(t^2\mathscr{L}_{\text{low}}(\nabla)v\Big),\end{aligned} \tag{1.12}$$

where for shortness we write $\mathscr{L} = \mathscr{L}\big(\nabla, \frac{1}{\varepsilon}\big)$ and define $\varphi_1(\gamma) = \gamma^{-1}(e^{\gamma}-1)$ for $\gamma \in \mathbf{C}$. Plugging (1.12) into (1.11) yields for a small time step τ that

$$\begin{aligned}u(\tau) = e^{i\tau\mathscr{L}}v - \tau i e^{i\tau\mathscr{L}}|\nabla|^{\alpha}\Big[p_{\text{low}}(v,\overline{v})\varphi_1\Big(i\tau\mathscr{L}_{\text{dom}}\Big(\nabla,\frac{1}{\varepsilon}\Big)\Big)p_{\text{dom}}(v,\overline{v})\Big] \\ + \mathcal{O}\Big(\tau^2|\nabla|^{2\alpha}\mathscr{L}_{\text{low}}(\nabla)q(u)\Big)\end{aligned} \tag{1.13}$$

for some polynomial q. The expansion of the exact solution (1.13) builds the foundation of the first-order resonance based discretiatzion

$$u^{n+1} = e^{i\tau\mathscr{L}}u^n - \tau i e^{i\tau\mathscr{L}}\Big[p_{\text{low}}(u^n,\overline{u}^n)\varphi_1\Big(i\tau\mathscr{L}_{\text{dom}}\Big(\nabla,\frac{1}{\varepsilon}\Big)\Big)p_{\text{dom}}(u^n,\overline{u}^n)\Big]. \tag{1.14}$$

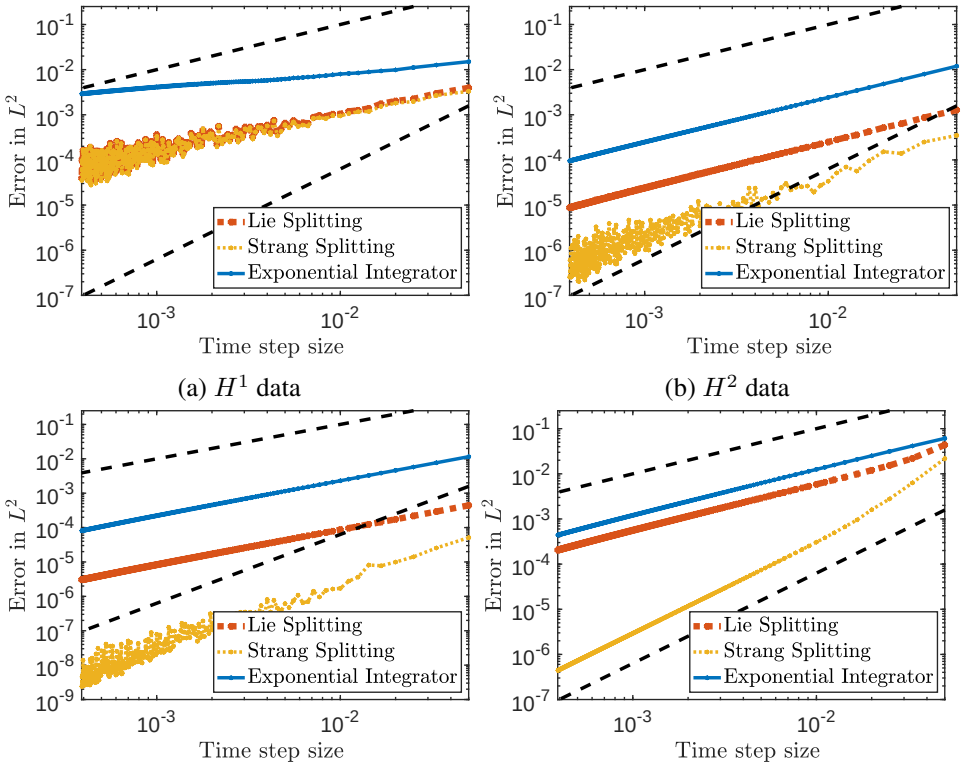
Compared to classical linear frequency approximations (cf. Table 1) the main gain of the more involved resonance based approach (1.14) is the following: All dominant parts $\mathscr{L}_{\text{dom}}$ are captured exactly in the discretisation, while only the lower order/non-oscillatory parts $\mathscr{L}_{\text{low}}$ are approximated. Henceforth, within the resonance based approach (1.14) the local error only depends on the lower order, non-oscillatory operator $\mathscr{L}_{\text{low}}$, while the local error of classical methods involve the full operator $\mathscr{L}$ and, in particular, its dominant part $\mathscr{L}_{\text{dom}}$. This allows us to obtain convergence for a more general class of solutions

$$\begin{aligned}u \in \underbrace{\mathscr{D}\Big(|\nabla|^{\alpha}\mathscr{L}_{\text{low}}\Big(\nabla,\frac{1}{\varepsilon}\Big)\Big)}_{\text{resonance domain}} \cap \mathscr{D}\big(|\nabla|^{2\alpha}\big) \\ \supset \mathscr{D}\Big(|\nabla|^{\alpha}\mathscr{L}\Big(\nabla,\frac{1}{\varepsilon}\Big)\Big) \cap \mathscr{D}\big(|\nabla|^{2\alpha}\big) = \underbrace{\mathscr{D}\Big(|\nabla|^{\alpha}\mathscr{L}_{\text{dom}}\Big(\nabla,\frac{1}{\varepsilon}\Big)\Big)}_{\text{classical domain}} \cap \mathscr{D}\big(|\nabla|^{2\alpha}\big).\end{aligned}$$

The particular construction of first-order resonance based schemes for the Schrödinger, Korteweg–de–Vries equation and the Klein–Gordon–Zakharov system is given in [4, 47, 67].

1.2 High order resonance based schemes

Classical approximation techniques, such as splitting or exponential integrator methods, can easily be extended to higher order, see, e.g., [43, 46, 74]. The step



(a) H^1 data (b) H^2 data

(c) H^3 data (d) $\mathscr{C}^\infty$ data

Figure 2: Order reduction of classical schemes in case of low regularity data (error versus step size for cubic Schrödinger equation). For smooth solutions classical methods reach their full order of convergence (lower right picture). In contrast, for less smooth solutions they suffer from severe order reduction (upper row). The initial values in H^1 and $\mathscr{C}^\infty$ are plotted in Figure 1. The slope of the dashed line is one (left and middle picture) and one and two, respectively (right picture).

from a first- to higher-order approximation lies in subsequently employing a higher order Taylor series expansion to the exact solution

$$u(t) = u(0) + t\partial_t u(0) + \ldots + \frac{t^r}{r!}\partial_t^r u(0) + \mathcal{O}\big(t^{r+1}\partial_t^{r+1} u\big). \tag{1.15}$$

Within this expansion, the higher order iterations of the oscillations (1.4) in the exact solution are, however, not resolved, but subsequently linearised. Therefore, classical high order methods are restricted to smooth solutions as their local approximation error $\mathcal{O}\big(t^{r+1}\partial_t^{r+1} u\big)$ involves high order derivatives. This phenomenon is also illustrated in Figure 2 where we numerically observe the order reduction of the Strang splitting method (of classical order two) down to the order of the Lie splitting method (of classical order one) in case of rough solutions.

At first glance the resonance based approach proposed in Section 1.1 can also be straightforwardly extended to higher order. Instead of considering only the first

order iteration (1.3) the idea is to iterate Duhamel's formula (1.2) up to the desired order r. Informally, the solution U^r up to order r can be represented by a series:

$$U^r(t,v) = \sum_{T\in\mathcal{V}^r} \frac{\Upsilon^p(T)}{S(T)}(\Pi T)(t,v), \tag{1.16}$$

where $\mathcal{V}$ is a set of decorated trees associated to the equation (1.1), $S(T)$ is the symmetry factor associated to the tree T, $\Upsilon^p(T)$ is the coefficient appearing in the iteration of the Duhamel's formulation and $(\Pi T)(t,v)$ represents an iterated integral. The precise definitions will be given in Section 4 below. Here $\mathcal{V}^r \subset \mathcal{V}$ denote the trees of size r which are the trees producing an iterated integral with r integrals.

The expansion (1.16) introduces a remainder of the desired order

$$\mathcal{O}\Big(\nabla^{(r+1)\alpha} t^{r+1} q(v)\Big)$$

for some polynomial q. The main difficulty then lies in devolping for every $T \in \mathcal{V}^r$ a suitable approximation to the iterated integrals $(\Pi T)(t,v)$ with the aim of minimising the local error structure (in the sense of regularity). In order to achieve this, the key idea is to embed, in the spirit of (1.9), the underlying resonance structure of the iterated integrals $(\Pi T)(t,v)$ into the discretisation. This is however much more involved than tackling the first-order oscillations (1.4) as for every tree $T \in \mathcal{V}^r$ its iterated nonlinear frequency interactions need to be controlled up to high order.

To compute these iterated frequency interactions the approximation is expressed in Fourier space. Therefore, one has to introduce extra decorations on the trees which encode the frequency. The $k-$th Fourier coefficient of (1.16) is given by

$$U^r_k(\tau,v) = \sum_{T\in\mathcal{V}^r_k} \frac{\Upsilon^p(T)(v)}{S(T)}(\Pi T)(\tau) \tag{1.17}$$

where Υ^p and Π are now defined on a different set of decorated trees $\mathcal{V}^r_k$ which incorporate the frequency k. The approximation of the previous sum is given by

$$U^{r,n}_k(\tau,v) = \sum_{T\in\mathcal{V}^r_k} \frac{\Upsilon^p(T)(v)}{S(T)}(\Pi^r_n T)(\tau) \tag{1.18}$$

where the map $\Pi^r_n T$ is an approximation of order r of the map ΠT in the sense that

$$(\Pi T - \Pi^r_n T)(\tau) = \mathcal{O}\big(\tau^{r+2}\mathcal{L}^r_{\text{low}}(T,n)\big). \tag{1.19}$$

Here $\mathcal{L}^r_{\text{low}}(T,n)$ involves all lower order frequency interactions that we neglect in our resonance based discretisation.

The approximation Π^r_n is constructed from a character Π_n defined on the vector space $\mathcal{H}$ spanned by decorated forests taking value in the space of trigonometric polynomials $\mathcal{C}$. The map Π_n is defined recursively from an operator $\mathcal{K}$ which will compute a suitable approximation (matching the regularity of the solution)

of the integrals introduced by the iteration of Duhamel's formula. This map $\mathscr{K}$ corresponds to the high order counterpart of the approach described in Section 1.1: it embeds the idea of singling out the dominant part and integrating it exactly while only approximating the lower order terms, allowing for an improved local error structure. The character Π_n is the main map for computing the numerical scheme in Fourier space. We will see that one can always map this scheme back to Physical space using classical operators.

In order to obtain a better understanding of the error introduced by the character Π_n, one needs to isolate each interaction. Therefore, we introduce two characters $\hat{\Pi}_n : \mathscr{H} \to \mathscr{C}$ and $A_n : \mathscr{H} \to \mathbf{C}$ such that

$$\Pi_n = \Big(\hat{\Pi}_n \otimes A_n\Big)\Delta \tag{1.20}$$

where $\Delta : \mathscr{H} \to \mathscr{H} \otimes \mathscr{H}_+$ is a coaction and $(\mathscr{H}, \Delta)$ is a right comodule for a Hopf algebra $\mathscr{H}_+$ equipped with a coproduct Δ^+ and an antipode $\mathscr{A}$. In fact, on can show that:

$$\hat{\Pi}_n = (\Pi_n \otimes (\mathbb{Q} \circ \Pi_n \mathscr{A} \cdot)(0))\Delta, \quad A_n = (\mathbb{Q} \circ \Pi_n \cdot)(0), \tag{1.21}$$

where Π_n is extended to a character on $\mathscr{H}_+$ and $\mathbb{Q}$ is a projection defined on $\mathscr{C}$ which keeps only the terms with no oscillations. The identity (1.20) can be understood as a Birkhoff type factorisation of $\hat{\Pi}_n$ using the character Π_n. This identity is also reminiscent in the main results obtained for singular SPDEs [12] where two twisted antipodes play a fundamental role providing a variant of the algebraic Birkhoff factorisation.

The coproduct Δ^+ and the co-action Δ are extremely close in spirit to the ones defined for the recentering in [44, 12]. Indeed, for designing a numerical scheme, we need to perform Taylor expansions and these two maps are performing them at the level of the algebra. The main difference with the tools used for singular SPDEs [12] is the length of the Taylor expansion which is now dictated by the order of the scheme. The structure, we propose in Section 2 is new and reveals the universality of deformed Butcher-Connes-Kreimer coproducts which appear in [12]. The non-deformed version of this map is coming from the analysis of B-series in [16, 26, 19], which is itself an extension of the Connes-Kreimer Hopf algebra of rooted trees [30, 31] arising in perturbative QFT and noncommutative geometry.

One can notice that our approximation Π_n^r depends on n which has to be understood as the regularity we assume a priori on the solution. We design our framework such that for smooth solutions the numerical schemes are simplified, recovering in the limit classical linearised approximations as in Table 1.

Remark 1.1 The term $\mathscr{L}^r_{\text{low}}(T, n)$ in the approximation (1.19) is obtained by performing several Taylor expansions. Depending on the value n, we get different numerical schemes (see also the applications in Appendix A). In the sequel, we focus on two specific values of n associated to two particular schemes. We consider

$n^r_{\text{low}}(T)$ and $n^r_{\text{exp}}(T)$ given by:

$$n^r_{\text{low}}(T) = \deg(\mathscr{L}^r_{\text{low}}(T)), \quad n^r_{\text{exp}}(T) = \deg(\mathscr{L}^r_{\text{exp}}(T)),$$

where $\mathscr{L}^r_{\text{low}}(T)$ corresponds to the error obtained when we integrate exactly the dominant part $\mathscr{L}_{\text{dom}}(T)$ and Taylor expand only the lower order part $\mathscr{L}_{\text{low}}(T)$, while the term $\mathscr{L}^r_{\text{exp}}(T)$ corresponds to the error one obtains when we Taylor expand the full operator $\mathscr{L}(T) = \mathscr{L}_{\text{dom}}(T) + \mathscr{L}_{\text{low}}(T)$. One has

$$\deg(\mathscr{L}^r_{\text{low}}(T,n)) = \begin{cases} n^r_{\text{low}}(T), & \text{if } n \leq n^r_{\text{low}}(T), \\ n, & \text{if } n^r_{\text{low}}(T) \leq n \leq n^r_{\text{exp}}(T), \\ n^r_{\text{exp}}(T), & \text{if } n \geq n^r_{\text{exp}}(T). \end{cases} \tag{1.22}$$

At the level of the scheme, we get

$$\Pi^r_n T = \begin{cases} \Pi^r_{\text{low}} T, & \text{if } n \leq n^r_{\text{low}}(T), \\ \Pi^r_n T, & \text{if } n^r_{\text{low}}(T) \leq n \leq n^r_{\text{exp}}(T), \\ \Pi^r_{\text{exp}} T, & \text{if } n \geq n^r_{\text{exp}}(T), \end{cases} \tag{1.23}$$

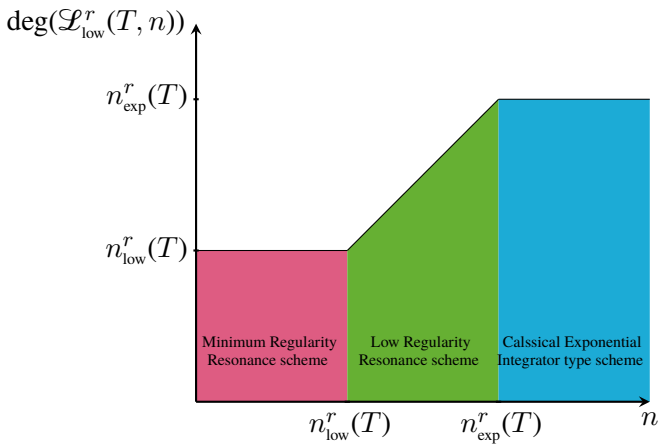
where we call $\Pi^r_{\text{low}} T$ the minimum regularity resonance based scheme. This scheme corresponds to the minimisation of the local-error and we can observe a plateau. Indeed, if n is too small then by convention we get this scheme. This could be the case if one does not compute the minimum regularity needed a priori.

The other scheme $\Pi^r_{\text{exp}} T$ corresponds to a classical exponential type discretisation, where enough regularity is assumed such that also the dominant components of the iterated integral can be expanded into a Taylor series as in (1.15). Then, we observe a second plateau: indeed assuming more regularity will not change the scheme as we have already Taylor-expanded all the components.

Compared to $\Pi^r_{\text{low}} T$ the scheme $\Pi^r_{\text{exp}} T$ is in general much simpler as no nonlinear frequency interactions are taken into account. This comes at the cost that a smaller class of equations can be solved as much higher regularity assumptions are imposed.

Between these two schemes, lies a large class of intermediate schemes $\Pi^r_n T$ which we call *low regularity resonance based schemes*. They take advantage of Taylor-expanding a bit more when more regularity is assumed. Therefore, the complexity of the schemes is decreasing as n increases see also Appendix A. We

can represent these different regimes through the diagram below.



Remark 1.2 Within our framework we propose a stabilisation technique. This will allow us to improve previous higher order attempts breaking formerly imposed order barriers of higher order resonance based schemes, such as the order barrier of $3/2$ observed for Schrödinger equations in [57]. Details are given in Remark 3.2 as well as Appendix A.

Remark 1.3 The aim is choose the central approximation $\Pi^r_n T$ as an interplay between optimising the local error in the sense of regularity while allowing for a practical implementation. We design our schemes in such a way that products of functions can always be mapped back to physical space. In practical computations, this will allow us to benefit from the Fast Fourier Transform (FFT) with computational effort of order $\mathcal{O}\big(|K|^d \log |K|^d\big)$ in dimension d, where K denotes the highest frequency in the discretisation. However, it comes at the cost that the approximation error (1.19) involves lower order derivatives. If, on the other hand, we would embed all nonlinear frequency interactions into the discretisation the resulting schemes would converge under weaker regularity assumptions, but they would be very restricted: only allowing first-order approximations in one spatial dimension for polynomial degrees of very low order. This is due to the fact that the time stepping would need to be carried out fully in Fourier space causing large memory and computational efforts of order $\mathcal{O}\big(K^{d\cdot \deg p}\big)$, where $\deg(p)$ denotes the degree of the nonlinearity p.

1.3 Outline of the paper

Let us give a short review of the content of this paper. In Section 2, we introduce the general algebraic framework by first defining a suitable vector space of decorated forests $\hat{\mathscr{H}}$. Next we define the dominant frequencies of a decorated forest (see Definition 2.5) and show that one can map them back into Physical space (see Corollary 2.9) which will be important for the efficiency of the numerical schemes (cf. Remark 1.3). Then, we introduced two spaces of decorated forests $\mathscr{H}_+$ and

$\mathcal{H}$. The latter $\mathcal{H}$ is used for describing approximated iterated integrals. The main difference with the previous space is that now we project along the order r of the method. We define the maps for the coaction $\Delta : \mathcal{H} \to \mathcal{H} \otimes \mathcal{H}_+$ and the coproduct $\Delta^+ : \mathcal{H}_+ \to \mathcal{H}_+ \otimes \mathcal{H}_+$ in (2.16) and (2.17). In addition we provide a recursive definition for them in (2.19). We prove in Proposition 2.15 that these maps give a right-comodule structure for $\mathcal{H}$ over the Hopf algebra $\mathcal{H}_+$. Moreover, we get a simple expression for the antipode $\mathcal{A}$ in Proposition 2.30.

In Section 3, we construct the approximation of the iterated integrals given by the character $\Pi : \hat{\mathcal{H}} \to \mathcal{C}$ (see (3.1)) through the character $\Pi_n : \mathcal{H} \to \mathcal{C}$ (see (3.2)). The main operator used for the recursive construction is $\mathcal{K}$ given in Definition 3.1. We introduce a new character $\hat{\Pi}_n : \mathcal{H} \to \mathcal{C}$ through a Birkhoff type factorisation obtained from the character Π_n (see Proposition 3.7). Thanks to $\hat{\Pi}_n$, we are able to conduct the local error analysis and show one of the main results of the paper: the error estimate on the difference between Π and its approximation Π_n (see Theorem 3.11). In Section 4, we introduce decorated trees stemming from Duhamel's formula via the rules formalism (see Definition 4.2). Then, we are able to introduce the general scheme (see Definition 4.12) and conclude on its local error structure (see Theorem 4.7).

In the Appendix A we illustrate the general framework on various applications and conclude in Section A.4 with numerical experiments underlying the favourable error behaviour of the new resonance based schemes for non-smooth, and in certain cases even for smooth, solutions.

Acknowledgements

First discussions on this work were initiated while the authors participated in the workshop "Algebraic and geometric aspects of numerical methods for differential equations" held at the Institut Mittag-Leffler in July 2018. The authors thank the organisers of this workshop for putting together a stimulating program bringing different communities together, and the members of the institute for providing a friendly working atmosphere. KS has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No. 850941).

2 General framework

2.1 Decorated trees and frequency interactions

We consider a set of decorated trees following the formalism developed in [12]. These trees will encode the Fourier coefficients of the numerical scheme.

We assume a finite set $\mathfrak{L}$ and $k_1, ..., k_n \in \mathbf{Z}^d$. We consider a family of polynomials $(P_\mathfrak{l})_{\mathfrak{l}\in\mathfrak{L}}$ indexed by this set. We define the set of decorated trees $\hat{\mathcal{T}}$ as elements of the form $T_\mathfrak{e}^{\mathfrak{n},\mathfrak{o}} = (T, \mathfrak{n}, \mathfrak{o}, \mathfrak{e})$ where

- T is a non-planar rooted tree with root ϱ_T, node set N_T and edge set E_T. We denote the leaves of T by L_T. T must also be a planted tree which means that there is only one edge outgoing the root.

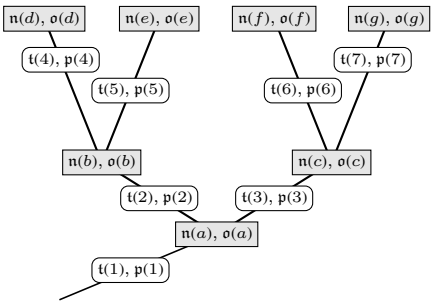
- the map $\mathfrak{e} : E_T \to \mathfrak{L} \times \{0,1\}$ are edge decorations.
- the map $\mathfrak{n} : N_T \setminus \{\varrho_T\} \to \mathbf{N}$ are node decorations.
- the map $\mathfrak{o} : N_T \setminus \{\varrho_T\} \to \mathbf{Z}^d$ are node decorations satisfying for every inner nodes u:

$$(-1)^{\mathfrak{p}(e_u)}\mathfrak{o}(u) = \sum_{e=(u,v)\in E_T} (-1)^{\mathfrak{p}(e)}\mathfrak{o}(v) \tag{2.1}$$

  where $\mathfrak{e}(e) = (\mathfrak{t}(e), \mathfrak{p}(e))$ and e_u is the edge outgoing u of the form (v,u) . From this definition, one can see that the node decorations $(\mathfrak{o}(u))_{u\in L_T}$ determine the decoration of the inner nodes. We assume that the node decorations at the leaves are linear combinations of the k_i with coefficients in $\{-1,0,1\}$.
- we assume that the root of T has no decoration.

When the node decoration $\mathfrak{n}$ is zero, we will denote the decorated trees $T_{\mathfrak{e}}^{\mathfrak{n},\mathfrak{o}}$ as $T_{\mathfrak{e}}^{\mathfrak{o}} = (T, \mathfrak{o}, \mathfrak{e})$. The set of decorated trees satisfying such condition is denoted by $\hat{\mathcal{T}}_0$. We say that $\bar{T}_{\bar{\mathfrak{e}}}^{\bar{\mathfrak{o}}}$ is a decorated subtree of $T_{\mathfrak{e}}^{\mathfrak{o}} \in \hat{\mathcal{T}}_0$ if $\bar{T}$ is a subtree of T and the restriction of the decorations $\mathfrak{o}, \mathfrak{e}$ of T to $\bar{T}$ are given by $\bar{\mathfrak{o}}$ and $\bar{\mathfrak{e}}$.

Example 1 Below, we give an example of a decorated tree $T_{\mathfrak{e}}^{\mathfrak{n},\mathfrak{o}}$ where the edges are labelled with numbers from 1 to 7 and the set $N_T \setminus \{\varrho_T\}$ is labelled by $\{a,b,c,d,e,f,g\}$:



Remark 2.1 The structure imposed on the node decorations (2.1) is close to the one used in [27, 41, 38]. But in these works, the trees were designed only for one particular equation. In our framework, we cover a general class of dispersive equations by having more decorations on the edges given by $\mathfrak{L} \times \{0,1\}$. The set $\mathfrak{L}$ keeps track of the differential operators in Duhamel's formulation. The second edge decoration allows us to compute an abstract conjugate on the trees given in (4.8).

We denote by $\hat{H}$ (resp. $\hat{H}_0$) the (unordered) forests composed of trees in $\hat{\mathcal{T}}$ (resp. $\hat{\mathcal{T}}_0$) (including the empty forest denoted by $\mathbf{1}$). Their linear spans are denoted by $\hat{\mathcal{H}}$ and $\hat{\mathcal{H}}_0$. We extend the definition of decorated subtree to forest by saying that T is a decorated subtree of the decorated forest F if their exists a decorated tree $\bar{T}$ in F such that T is decorated subtree of $\bar{T}$. The forest product is denoted by $\cdot$ and the counit is $\mathbf{1}^\star$ which is non-zero only on the empty forest.

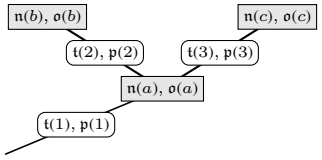
In order to represent these decorated trees, we introduce a symbolic notation. An edge decorated by $o = (\mathfrak{t}, \mathfrak{p})$ is denoted by $\mathcal{I}_o$. The symbol $\mathcal{I}_o(X_k^\ell \cdot) : \hat{\mathscr{H}} \to \hat{\mathscr{H}}$ is viewed as the operation that merges all the roots of the trees composing the forest into one node decorated by $(\ell, k) \in \mathbf{N} \times \mathbf{Z}^d$. We obtain a decorated tree which is then grafted onto a new root with no decoration. If the condition (2.1) is not satisfies on the argument then $\mathcal{I}_o(X_k^\ell \cdot)$ gives zero. If $\ell = 0$, then the term X_k^ℓ is denoted by X_k as a short hand notation for X_k^0. When $\ell = 1$, it will be denoted by X_k^1. The forest product between $\mathcal{I}_{o_1}(X_{k_1}^{\ell_1} T_1)$ and $\mathcal{I}_{o_2}(X_{k_2}^{\ell_2} T_2)$ is given by:

$$\mathcal{I}_{o_1}(X_{k_1}^{\ell_1} T_1)\mathcal{I}_{o_2}(X_{k_2}^{\ell_2} T_2) := \mathcal{I}_{o_1}(X_{k_1}^{\ell_1} T_1) \cdot \mathcal{I}_{o_2}(X_{k_2}^{\ell_2} T_2).$$

Example 2 The following symbol

$$\mathcal{I}_{(\mathfrak{t}(1),\mathfrak{p}(1))}(X_{\mathfrak{o}(a)}^{\mathfrak{n}(a)} \mathcal{I}_{(\mathfrak{t}(2),\mathfrak{p}(2))}(X_{\mathfrak{o}(b)}^{\mathfrak{n}(b)}) \mathcal{I}_{(\mathfrak{t}(3),\mathfrak{p}(3))}(X_{\mathfrak{o}(c)}^{\mathfrak{n}(c)}))$$

encodes the tree



(2.2)

We will see later (in Example 3) that the above tree with suitable chosen decorations describes the first iterated integral of the Kortweg–de Vries equation (A.30).

We are interested in the following quantity which represents the frequency associated to this tree:

$$\mathcal{R}(T_{\mathfrak{e}}^{\mathfrak{o}}) = \sum_{u \in N_T} P_{(\mathfrak{t}(e_u),\mathfrak{p}(e_u))}(\mathfrak{o}(u)) \tag{2.3}$$

where e_u is the edge outgoing u of the form (v, u) and

$$P_{(\mathfrak{t}(e_u),\mathfrak{p}(e_u))}(\mathfrak{o}(u)) = (-1)^{\mathfrak{p}(e_u)} P_{\mathfrak{t}(e_u)}((-1)^{\mathfrak{p}(e_u)} \mathfrak{o}(u)). \tag{2.4}$$

The term $\mathcal{R}(T_{\mathfrak{e}}^{\mathfrak{o}})$ has to be understood as a polynomial in multiple variables given by the k_i.

In the numerical scheme what matters are the terms with maximal degree of frequency which are here the monomials of higher degree, cf. $\mathscr{L}_{\text{dom}}$. We compute them using the symbolic notation in the next section. We assume fixed $\mathfrak{L}_+ \subset \mathfrak{L}$.

2.2 Dominant parts of trees and physical space maps

Definition 2.2 Let $P(k_1, ..., k_n)$ a polynomial in the k_i. If the higher monomials of P are of the form

$$a\sum_{i=1}^{n}(a_i k_i)^m, \quad a_i \in \{-1, 0, 1\},\, a \in \mathbf{Z}$$

we define $\mathscr{P}_{\text{dom}}(P)$ as

$$\mathscr{P}_{\text{dom}}(P) = a\left(\sum_{i=1}^{n} a_i k_i\right)^m. \tag{2.5}$$

Otherwise, it is zero.

Remark 2.3 Terms of type (2.5) will naturally arise when filtering out the dominant nonlinear frequency interactions in the PDE. We have to embed integrals over their exponential into our discretisation. For their practical implementation it will be therefore essential to map fractions of (2.5) back to Physical space.

Indeed, if we apply the inverse Fourier transform $\mathscr{F}^{-1}$ one gets:

$$\begin{aligned}\mathscr{F}^{-1}&\left(\sum_{\substack{0\neq k=k_1+...+k_n\\ k_\ell\neq 0}} \frac{1}{(k_1+...+k_n)^m}\frac{1}{k_1^{m_1}}...\frac{1}{k_n^{m_n}} v_{k_1}^1...v_{k_n}^n e^{ikx}\right)\\ &= (-\Delta)^{-m/2}\prod_{\ell=1}^{n}\left((-\Delta)^{-m_\ell/2}v^\ell(x)\right)\end{aligned}$$

where by abuse of notation we define the operator $(-\Delta)^{-1}$ in Fourier space as $(-\Delta)^{-1}f(x) = \sum_{k\neq 0}\frac{\hat{f}_k}{k^2}e^{ikx}$.

Proposition 2.4 *Assume that we have polynomials Q in $k_1, \ldots, k_n$ and k is a linear combination of the k_i such that:*

$$\begin{aligned}Q &= \prod_j (\sum_{u\in V_j} a_{u,V_j}k_u)^{m_i}, \quad V_j \subset \{1, ..., n\}, \quad a_{u,V_j} \in \{-1, 1\}\\ k &= \sum_{u=1}^{n} a_u k_u, \quad a_i \in \{-1, 1\}\end{aligned}$$

where the V_i are either disjoint or if $V_j \subset V_i$ we assume that there exist $p_{i,j}$ such that

$$a_{u,V_i} = (-1)^{p_{i,j}} a_{u,V_j}, \quad u \in V_j.$$

We also suppose that the V_i are included in k in the sense that there exist p_{V_i} such that

$$a_u = (-1)^{p_{V_i}} a_{u,V_i}, \quad u \in V_i.$$

Then, one gets

$$\mathscr{F}^{-1}\left(\sum_{\substack{0\neq k=a_1k_1+\ldots+a_nk_n \\ Q(k_1,\ldots,k_n)\neq 0}} \frac{1}{Q} v_{k_1}^{1,a_1}\ldots v_{k_n}^{n,a_n} e^{ikx} \right) = \left(\prod_{V_i\subset V_j} (-1)^{p_{V_i}} (-\Delta)_{V_i}^{-m_i/2} \right) v^{1,a_1}\ldots v^{n,a_n}$$

where $v^{i,1} = v^i$ and $v^{i,-1} = \overline{v^i}$. The operators $(-\Delta)_{V_i}^{-m_i/2}$ acts only on the functions $\prod_{u\in V_i} v^{u,a_u}$ and the product starts by the smaller elements for the inclusion order.

Proof. We proceed by induction on the number of V_i. Let $V_{\max}$ an element among the V_i maximum for the inclusion order. Then, we get

$$\sum_{\substack{0\neq k=a_1k_1+\ldots+a_nk_n \\ Q(k_1,\ldots,k_n)\neq 0}} \frac{1}{Q} v_{k_1}^{1,a_1}\ldots v_{k_n}^{n,a_n} e^{ikx} = \sum_{\substack{0\neq k=r+\ell \\ \ell\neq 0}} \frac{(-1)^{p_{V_{\max}}}}{\ell^{m_{\max}}} \sum_{\substack{0\neq r=\sum_{u\notin V_{\max}} a_u k_u \\ R\neq 0}} \frac{1}{R} \left(\prod_{j\notin V_{\max}} v_{k_j}^{j,a_j} \right) e^{irx} \times \sum_{\substack{0\neq \ell=\sum_{u\in V_{\max}} a_u k_u \\ S\neq 0}} \frac{1}{S} \left(\prod_{j\in V_{\max}} v_{k_j}^{j,a_j} \right) e^{i\ell x}$$

where

$$S = \prod_{V_j\subsetneq V_{\max}} \Big(\sum_{u\in V_j} a_{u,V_j} k_u\Big)^{m_i}, \quad R = \prod_{V_j\cap V_{\max}=\emptyset} \Big(\sum_{u\in V_j} a_{u,V_j} k_u\Big)^{m_i}, \quad Q = RS\ell^{m_{max}}.$$

Thus, by applying the inverse Fourier transform, we get the term $(-1)^{p_{V_{\max}}}(-\Delta)_{V_{\max}}^{-m_{\max}/2}$ from $\frac{(-1)^{p_{V_{\max}}}}{\ell^{m_{\max}}}$. We conclude from the induction hypothesis on the two remaining sums. □

Definition 2.5 We recursively define $\mathscr{R}_{\text{dom}}, \mathscr{R}_{\text{low}} : \hat{H}_0 \to \mathbf{Z}^d$ as:

$$\mathscr{R}_{\text{dom}}(\mathbf{1}) = 0 \quad \mathscr{R}_{\text{dom}}(T\cdot\bar{T}) = \mathscr{R}_{\text{dom}}(T) + \mathscr{R}_{\text{dom}}(\bar{T})$$
$$\mathscr{R}_{\text{dom}}(\mathscr{I}_{(\mathfrak{t},\mathfrak{p})}(X_k T)) = \begin{cases} \mathscr{P}_{\text{dom}}(P_{(\mathfrak{t},\mathfrak{p})}(k) + \mathscr{R}_{\text{dom}}(T)), \text{ if } \mathfrak{t}\in\mathfrak{L}_+, \\ P_{(\mathfrak{t},\mathfrak{p})}(k) + \mathscr{R}_{\text{dom}}(T), \quad \text{otherwise} \end{cases}$$
$$\mathscr{R}_{\text{low}}(\mathscr{I}_{(\mathfrak{t},\mathfrak{p})}(X_k T)) = (\text{id} - \mathscr{P}_{\text{dom}})(P_{(\mathfrak{t},\mathfrak{p})}(k) + \mathscr{R}_{\text{dom}}(T)).$$

We extend these two maps to $\hat{H}$ by ignoring the node decorations $\mathfrak{n}$.

Remark 2.6 The definition of $\mathscr{P}_{\text{dom}}$ can be adapted depending on what is considered to be the dominant part. For example, if for $\mathfrak{t}_2 \in \mathfrak{L}_+$, one has (cf. (1.7)):

$$P_{(\mathfrak{t}_2,p)}(X) = \frac{1}{\varepsilon^\sigma} + F_{(\mathfrak{t}_2,p)}(X)$$

and we can define the dominant part only depending on ε (see Example A.3)

$$\mathscr{P}_{\text{dom}}(P_{(\mathfrak{t}_2,p)}(k)) = \frac{1}{\varepsilon^\sigma}.$$

Remark 2.7 The set $\mathfrak{L}_+$ encodes integration in time, see also its interpretation given in (3.1) below. On the other hand, the set $\mathfrak{L}_-$ corresponds in practice to the change of variable performed in Duhamel's formulation.

The map $\mathscr{R}_{\text{dom}}$ has a nice property regarding the tree inclusions given in the next proposition. This inclusive property will be important in practical computations, see also Remark 1.3 and the examples in Appendix A.

Proposition 2.8 *Let $F = T^{\mathfrak{o}}_{\mathfrak{e}}$ be a decorated forest in $\hat{H}_0$ and $e \in E_T$. We consider the decorated subtree $(T_e)^{\mathfrak{o}}_{\mathfrak{e}}$ where T_e corresponds to the tree above e. The nodes of T_e are given by all the nodes whose path to the root contains e. Then, one has*

$$\mathscr{P}_{dom}(\mathscr{R}_{dom}(T^{\mathfrak{o}}_{\mathfrak{e}})) = a \sum_{u\in V} (a_u k_u)^m, \quad a \in \mathbf{Z},\, V \subset L_T,\, a_u \in \{-1,1\} \tag{2.6}$$
$$\mathscr{P}_{dom}(\mathscr{R}_{dom}((T_e)^{\mathfrak{o}}_{\mathfrak{e}})) = b \sum_{u\in \bar{V}} (b_u k_u)^m, \quad b \in \mathbf{Z},\, \bar{V} \subset L_T,\, b_u \in \{-1,1\}$$

and $\bar{V} \subset V$ or $\bar{V} \cap V = \emptyset$. If $\bar{V} \subset V$, then there exists $\bar{p} \in \{0,1\}$ such that $a_u = (-1)^{\bar{p}} b_u$ for every $u \in \bar{V}$. Moreover, for $F = \prod_i T_i$ where the T_i are decorated trees with root ϱ_i, there exists p such that

$$\sum_i (-1)^{p_i} \mathfrak{o}(v_i) = \sum_{u\in L_T} (c_u k_u), \quad c_u = (-1)^p a_u, \quad u \in V \tag{2.7}$$

where $e_i = (\varrho_i, v_i) \in E_T$ and $\mathfrak{e}(e_i) = (\mathfrak{t}_i, p_i)$.

Proof. We proceed by induction on the size of the forest.

(i) If $F = \prod_i T_i$ then one has:

$$\mathscr{P}_{\text{dom}}(\mathscr{R}_{\text{dom}}(F)) = \mathscr{P}_{\text{dom}}\left(\sum_i \mathscr{P}_{\text{dom}}(\mathscr{R}_{\text{dom}}(T_i))\right)$$

Then, we notice that $N_F = \sqcup_i N_{T_i}$ and we can apply the induction hypothesis on each of the T_i in order to conclude.

(ii) If $F = \mathscr{I}_{(\mathfrak{t},\mathfrak{p})}(X_k \bar{T})$ then

$$\mathscr{P}_{\text{dom}}(\mathscr{R}_{\text{dom}}(F)) = \mathscr{P}_{\text{dom}}\big(P_{(\mathfrak{t},\mathfrak{p})}(k) + \mathscr{R}_{\text{dom}}(\bar{T})\big)$$

$$= \mathscr{P}_{\text{dom}}\big(P_{(\mathfrak{t},\mathfrak{p})}(k) + \mathscr{P}_{\text{dom}}\big(\mathscr{R}_{\text{dom}}(\bar{T})\big)\big)$$

We apply the induction hypothesis on $\bar{T}$ (cf. (2.7)) and we get

$$\mathscr{P}_{\text{dom}}\big(\mathscr{R}_{\text{dom}}(\bar{T})\big) = a\sum_{u\in V}(a_u k_u)^m, \quad a \in \mathbf{Z},\ V \subset L_T,\ a_u \in \{-1,1\} \tag{2.8}$$
$$k = \sum_{u\in L_T}(c_u k_u), \quad c_u = (-1)^p a_u, \quad u \in V.$$

If the degree of $P_{(\mathfrak{t},\mathfrak{p})}(k)$ is higher than the degree of $\mathscr{R}_{\text{dom}}(\bar{T})$ we obtain that

$$\mathscr{P}_{\text{dom}}\big(P_{(\mathfrak{t},\mathfrak{p})}(k) + \mathscr{R}_{\text{dom}}(\bar{T})\big) = \mathscr{P}_{\text{dom}}(P_{(\mathfrak{t},\mathfrak{p})}(k)).$$

On the other hand, if the degree of $P_{(\mathfrak{t},\mathfrak{p})}(k)$ is lower than the degree of $\mathscr{R}_{\text{dom}}(\bar{T})$

$$\mathscr{P}_{\text{dom}}\big(P_{(\mathfrak{t},\mathfrak{p})}(k) + \mathscr{R}_{\text{dom}}(\bar{T})\big) = \mathscr{P}_{\text{dom}}\big(\mathscr{R}_{\text{dom}}(\bar{T})\big).$$

If $P_{(\mathfrak{t},\mathfrak{p})}(k)$ and $\mathscr{R}_{\text{dom}}(\bar{T})$ have the same degree m, we get using the definition of $P_{(\mathfrak{t},\mathfrak{p})}(k)$ in (2.4) as well as the induction hypothesis on k given in (2.8) that

$$\mathscr{P}_{\text{dom}}(P_{(\mathfrak{t},\mathfrak{p})}(k)) + \mathscr{P}_{\text{dom}}\big(\mathscr{R}_{\text{dom}}(\bar{T})\big) = \sum_{u\in V}\big(a(-1)^{p+m+\mathfrak{p}} + (-1)^{\mathfrak{p}}\big)((-1)^{\mathfrak{p}}c_u k_u)^m$$
$$+ \sum_{u\in L_T\setminus V}(-1)^{\mathfrak{p}}((-1)^{\mathfrak{p}}c_u k_u)^m + R$$

where R are terms of lower order.

By applying the map $\mathscr{P}_{\text{dom}}$ defined in (2.5), we thus obtain an expression of the form

$$\mathscr{P}_{\text{dom}}(\mathscr{R}_{\text{dom}}(F)) = b\left(\sum_{u\in\tilde{V}}(-1)^{\mathfrak{p}}c_u k_u\right)^m \text{ for some } b \in \mathbf{Z} \tag{2.9}$$

where $\tilde{V}$ could be either L_T or $L_T \setminus V$. Then, we obtain (2.7) because in all possible cases, one has $\tilde{V} \subset L_T$.

Let $e \in E_T$, $T_e \neq T$, then T_e is a subtree of $\bar{T}$. By the induction hypothesis, one obtains (2.6), meaning that if we denote by V (resp. $\bar{V}$) the set associated to $\bar{T}$ (resp. T_e), we get: $\bar{V} \subset V$ or $\bar{V} \cap V = \emptyset$.

In the first case $\bar{V} \subset V$, the assertion follows as $V \subset \tilde{V}$ or $V \cap \tilde{V} = \emptyset$ such that necessarily $\bar{V} \subset \tilde{V}$ or $\bar{V} \cap \tilde{V} = \emptyset$.

In the second case $\bar{V} \cap V = \emptyset$, we apply the induction hypothesis on T_e (cf (2.7)). Then, for v of T_e, there exists p such that the decoration $\mathfrak{o}(v)$ is given by:

$$\mathfrak{o}(v) = \sum_{u\in L_{T_v}}(d_u k_u), \quad d_u = (-1)^p b_u, \quad u \in \bar{V}.$$

As $\mathfrak{o}(v)$ appears as a subfactor in k, one has $\bar{V} \subset L_T$. Then, $\bar{V} \cap V = \emptyset$ gives also that $\bar{V} \subset L_T \setminus V$. Therefore, we have $\bar{V} \subset \tilde{V}$ which concludes the proof. □

Corollary 2.9 *Let $T^{\mathfrak{o}}_{\mathfrak{c}}$ a decorated tree in $\hat{\mathcal{T}}_0$. We assume a set A of decorated subtrees of $T^{\mathfrak{o}}_{\mathfrak{c}}$ such that $\mathscr{R}_{dom}(\bar{T}) \neq 0$ for $\bar{T} \in A$. Moreover, we assume that the $\bar{T}$ are of the form $(T_e)^{\mathfrak{o}}_{\mathfrak{c}}$ where $e \in E_T$. Then, the following product*

$$\prod_{\bar{T} \in A} \frac{1}{\big(\mathscr{R}_{dom}(\bar{T})\big)^{m_T}}$$

can be mapped back to Physical space using operators of the form $(-\Delta)_V^{-m/2}$ as defined in Proposition 2.4.

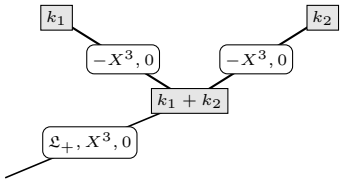
Proof. Proposition 2.8 gives us the structure needed for applying Proposition 2.4 which allows us to conclude. □

In the following we compute the dominant part $\mathscr{R}_{\text{dom}}$ for the underlying trees of the Schrödinger and Kortweg–de Vries (KdV) equation.

Example 3 (KdV) We consider the decorated tree T given in Example 2.2, where we fix the following decorations:

$$\mathfrak{p}(1) = \mathfrak{p}(2) = \mathfrak{p}(3) = 0, \quad \mathfrak{t}(2) = \mathfrak{t}(3) = \mathfrak{t}_2, \mathfrak{t}(1) = \mathfrak{t}_1$$
$$\mathfrak{o}(b) = k_1, \quad \mathfrak{o}(c) = k_2, \quad \mathfrak{o}(a) = k_1 + k_2, \quad P_{\mathfrak{t}_1}(X) = X^3, \quad P_{\mathfrak{t}_2}(X) = -X^3$$

Now, we suppose $\mathfrak{L}_+ = \{\mathfrak{t}_1\}$ and $\mathfrak{L} = \{\mathfrak{t}_1, \mathfrak{t}_2\}$. Then the tree (2.2) takes the form



(2.10)

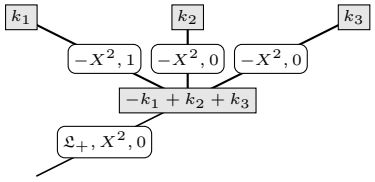
This tree corresponds to the first iterated integral for the KdV equation (A.30). Together with Definition 2.5 one gets

$$\begin{aligned}\mathscr{R}_{\text{dom}}(T) &= 0\\ \mathscr{R}_{\text{low}}(T) &= \mathscr{P}_{\text{dom}}\big((k_1+k_2)^3 - k_1^3 - k_2^3\big)\\ &= 3(k_1+k_2)(k_1+k_3)(k_2+k_3).\end{aligned}$$

Example 4 (Cubic Schrödinger) Next we consider the Symbol

$$\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{-k_1+k_2+k_3}\mathcal{I}_{(\mathfrak{t}_2,1)}(X_{k_1})\mathcal{I}_{(\mathfrak{t}_2,0)}(X_{k_2})\mathcal{I}_{(\mathfrak{t}_2,0)}(X_{k_3}))$$

with $P_{\mathfrak{t}_1}(X) = X^2$, $P_{\mathfrak{t}_2}(X) = -X^2$, $\mathfrak{L}_+ = \{\mathfrak{t}_1\}$ and $\mathfrak{L} = \{\mathfrak{t}_1, \mathfrak{t}_2\}$ which encodes the tree



(2.11)

This tree corresponds to the frequency interaction of the first iterated integral for the cubic Schrödinger equation (A.1). With Definition 2.5, we get

$$\begin{aligned}\mathscr{R}_{\text{dom}}(T) &= \mathscr{P}_{\text{dom}}\big((-k_1+k_2+k_3)^2+(-k_1)^2-k_2^3-k_3^3\big)\\ &= \mathscr{P}_{\text{dom}}\big(2k_1^2-2k_1(k_2+k_3)+2k_2k_3\big) = 2k_1^2\\ \mathscr{R}_{\text{low}}(T) &= (-k_1+k_2+k_3)^2+(-k_1)^2-k_2^3-k_3^3-2k_1^2\\ &= -2k_1(k_2+k_3)+2k_2k_3.\end{aligned}$$

2.3 Approximated decorated trees

We denote by $\mathscr{T}$ the set of decorated trees $T^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e},r} = (T,\mathfrak{n},\mathfrak{o},\mathfrak{e},r)$ where

- $T^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e}} \in \hat{\mathscr{T}}$.
- The decoration of the root is given by $r \in \mathbf{Z}$, $r \geq -1$ such that

$$r+1 \geq \deg(T^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e}}) \tag{2.12}$$

  where deg is defined recursively by

$$\begin{aligned}\deg(T_1\cdot T_2) &= \max(\deg(T_1),\deg(T_2))\\ \deg(\mathscr{I}_{(\mathfrak{t},\mathfrak{p})}(X_k^\ell T_1)) &= \ell + \mathbf{1}_{\{\mathfrak{t}\in\mathscr{L}_+\}} + \deg(T_1)\end{aligned}$$

  and T_1, T_2 are forests composed of trees in $\mathscr{T}$. The quantity $\deg(T^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e}})$ is the maximum number of edges with type in $\mathfrak{L}_+$ and node decorations $\mathfrak{n}$ lying on the same path from one leaf to the root.

Example 2 (Continued) We continue Example 2 with the decorated tree $T^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e}}$ given (2.2). We also suppose that $\mathfrak{t}_1$ is in $\mathscr{L}_+$ but not $\mathfrak{t}_2$. Then, one has

$$\deg(T^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e}}) = \mathfrak{n}(a)+1+\max(\mathfrak{n}(b),\mathfrak{n}(c)).$$

We denote by $\mathscr{H}$ the vector space spanned by forests composed of trees in $\mathscr{T}$ and X^n, $n \in \mathbf{N}$ where X^n is the tree with one node decorated by n. When the decoration n is equal to zero we identify this tree with the empty forest: $X^0 = \mathbf{1}$. Using the symbolic notation, one has:

$$\mathscr{H} = \langle\{\prod_j X^{m_j}\prod_i \mathscr{I}^{r_i}_{o_i}(X^{\ell_i}_{k_i}T_i),\ \mathscr{I}_{o_i}(X^{\ell_i}_{k_i}T_i)\in\hat{\mathscr{T}}\}\rangle$$

where the product used is the forest product. The map $\mathscr{I}^r_o(X^\ell_k\cdot):\hat{\mathscr{H}}\to\mathscr{H}$ is defined as the same as for $\mathscr{I}_o(X^\ell_k\cdot)$ except now the root is decorated by r and it could be zero if the inequality (2.12) is not satisfied. We extend this map to $\mathscr{H}$ by:

$$\mathscr{I}^r_o(X^\ell_k(\prod_j X^{m_j}\prod_i \mathscr{I}^{r_i}_{o_i}(X^{\ell_i}_{k_i}T_i))) = \mathscr{I}^r_o(X_k^{\ell+\sum_j m_j}(\prod_i \mathscr{I}_{o_i}(X^{\ell_i}_{k_i}T_i))).$$

In the extension, we remove the decorations r_i and we add up the decorations m_j with ℓ. In the sequel, we will use a recursive formulation and move from $\hat{\mathscr{H}}$ to $\mathscr{H}$.

Therefore, we define the map $\mathcal{D}_r : \hat{\mathcal{H}} \to \mathcal{H}$ which replaces the root decoration of a decorated tree by r and performs the projection along the identity (2.12). It is given by

$$\mathcal{D}_r(X^\ell) = \mathbf{1}_{\{\ell \leq r+1\}} X^\ell, \quad \mathcal{D}_r\Big(\mathcal{I}_o(X_k^\ell T)\Big) = \mathcal{I}_o^r(X_k^\ell T) \tag{2.13}$$

and we extend it multiplicatively to any forest in $\hat{\mathcal{H}}$.

Remark 2.10 The value r corresponds to the order of the scheme. This order must be higher than the maximum number of iterated integrations and polynomials lying on the same path from one leaf to the root. Moreover, we can only have polynomials of degree less than $r+1$ for an error of order $r+2$.

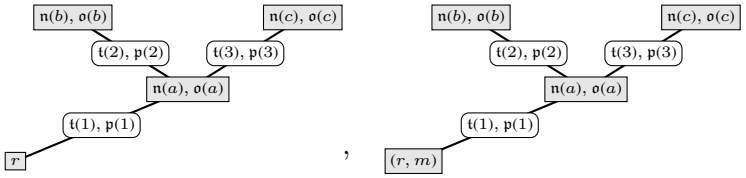
We denote by $\mathcal{T}_+$ the set of decorated forests composed of trees of the form $(T, \mathfrak{n}, \mathfrak{o}, \mathfrak{e}, (r, m))$ where

- $T_{\mathfrak{e},r}^{\mathfrak{n},\mathfrak{o}} \in \mathcal{T}$.
- The edge connecting the root has a decoration of the form $(\mathfrak{t}, \mathfrak{p})$ where $\mathfrak{t} \in \mathfrak{L}_+$.
- The decoration (r, m) is at the root of T and $m \in \mathbf{N}$ is such that $m \leq r+1$.

The linear span of $\mathcal{T}_+$ is denoted by $\mathcal{H}_+$. We can define the same grafting operator as before $\mathcal{I}_o^{(r,m)}(X_k^\ell \cdot) : \mathcal{H} \to \mathcal{H}_+$ as the same as $\mathcal{I}_o^r(X_k^\ell \cdot) : \mathcal{H} \to \mathcal{H}$ but now we add the decoration (r, m) at the root where $m \leq r+1$. We also define $\hat{\mathcal{D}}_{(r,m)} : \hat{\mathcal{H}} \to \mathcal{H}_+$ as the same as $\mathcal{D}_r$. It is given by

$$\hat{\mathcal{D}}_{(r,m)}(X^\ell) = \mathbf{1}_{\ell=0}, \quad \hat{\mathcal{D}}_{(r,m)}\Big(\mathcal{I}_o(X_k^\ell T)\Big) = \mathcal{I}_o^{(r,m)}(X_k^\ell T) \tag{2.14}$$

Example 2 (Continued) For the tree (2.2) we obtain when applying $\mathcal{D}_r$ and $\hat{\mathcal{D}}_{(r,m)}$



(2.15)

2.4 Operators on approximated decorated forests

We define a map $\Delta : \mathcal{H} \to \mathcal{H} \otimes \mathcal{H}_+$ for a given $T_{\mathfrak{e},r}^{\mathfrak{n},\mathfrak{o}} \in \mathcal{T}$ by

$$\begin{aligned}
\Delta T_{\mathfrak{e},r}^{\mathfrak{n},\mathfrak{o}} &= \sum_{A \in \mathfrak{A}(T)} \sum_{\mathfrak{e}_A} \frac{1}{\mathfrak{e}_A!} (A, \mathfrak{n} + \pi \mathfrak{e}_A, \mathfrak{o}, \mathfrak{e}, r) \\
&\quad \otimes \prod_{e \in \partial(A,T)} (T_e, \mathfrak{n}, \mathfrak{o}, \mathfrak{e}, (r - \deg(e), \mathfrak{e}_A(e))) \,, \\
&= \sum_{A \in \mathfrak{A}(T)} \sum_{\mathfrak{e}_A} \frac{1}{\mathfrak{e}_A!} A_{\mathfrak{e},r}^{\mathfrak{n}+\pi\mathfrak{e}_A,\mathfrak{o}} \otimes \prod_{e \in \partial(A,T)} (T_e)_{\mathfrak{e},(r-\deg(e),\mathfrak{e}_A(e))}^{\mathfrak{n},\mathfrak{o}}
\end{aligned} \tag{2.16}$$

where we use the following notations.

- Factorials coefficients are understood in multiindex notation.
- In $A^{\mathfrak{n}+\pi\mathfrak{e}_A,\mathfrak{o}}_{\mathfrak{e},r}$, the maps $\mathfrak{n}$, $\mathfrak{o}$ and $\mathfrak{e}$ are restricted to N_A and E_A. The same is valid for $(T_e)^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e},(r-\deg(e),\mathfrak{e}_A(e))}$ where the restriction is on $N_{T_e} \setminus \{\varrho_{T_e}\}$ and E_{T_e}, ϱ_{T_e} is the root of T_e.
- The first sum runs over $\mathfrak{A}(T)$, the set of all subtrees A of T containing the root ϱ of T. The second sum runs $\mathfrak{e}_A : \partial(A,T) \to \mathbf{N}$ where $\partial(A,T)$ denotes the edges in $E_T \setminus E_A$ of type in $\mathfrak{L}_+$ that are adjacent to N_A.
- We write T_e as the planted tree above the edge e in T. For $g : E_T \to \mathbf{N}$, we define for every $x \in N_T$, $(\pi g)(x) = \sum_{e=(x,y)\in E_T} g(e)$.
- We define $\deg(e)$ for $e \in E_T$ as the number of edges having $\mathfrak{t}(e) \in \mathfrak{L}_+$ lying on the path from e to the root in the decorated tree $T^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e}}$. We also add up the decoration $\mathfrak{n}$ on this path.

The map Δ is compatible toward the projection induced by the decoration r. Indeed, one has

$$\deg(T^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e}}) = \max_{e\in E_T} \left(\deg((T_e)^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e}}) + \deg(e)\right).$$

Therefore, if $\deg(T^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e}}) < r$ then for every $e \in E_T$

$$\deg((T_e)^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e}}) + \deg(e) < r.$$

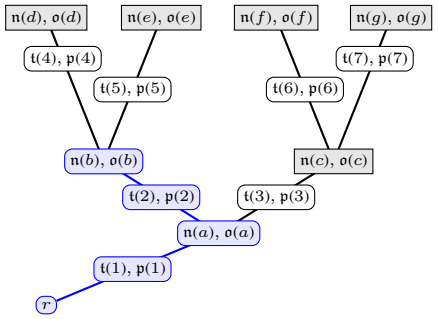
We deduce that if $T^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e},r}$ is zero then the $(T_e)^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e},(r-\deg(e),\mathfrak{e}_A(e))}$ are zero too.

We define a map $\Delta^+ : \mathscr{H}_+ \to \mathscr{H}_+ \otimes \mathscr{H}_+$ given for $T^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e},(r,m)} \in \mathscr{T}_+$ by

$$\Delta^+ T^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e},(r,m)} = \sum_{A\in\mathfrak{A}(T)} \sum_{\mathfrak{e}_A} \frac{1}{\mathfrak{e}_A!} A^{\mathfrak{n}+\pi\mathfrak{e}_A,\mathfrak{o}}_{\mathfrak{e},(r,m)} \otimes \prod_{e\in\partial(A,T)} (T_e)^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e},(r-\deg(e),\mathfrak{e}_A(e))} \quad (2.17)$$

We illustrate this coproduct on a well-chosen example.

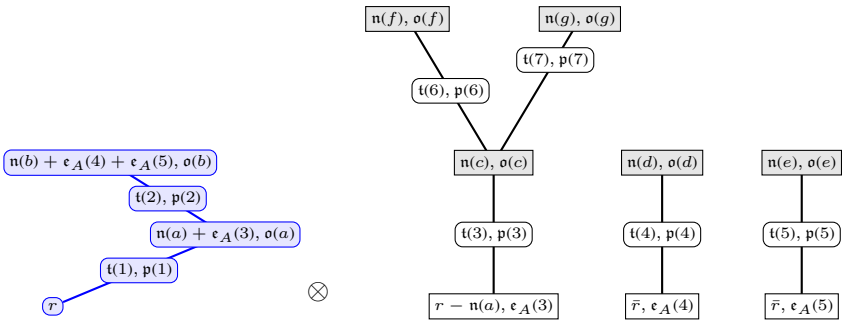
Example 1 (Continued) We continue with the tree in Example 1. We suppose that $\mathfrak{t}(3), \mathfrak{t}(4)$ and $\mathfrak{t}(5)$ belong to $\mathfrak{L}_+$. Below, the subtree $A \in \mathfrak{A}(T)$ is colored in blue. We have $N_A = \{\varrho, a, b\}$, $E_A = \{1, 2\}$ and $\partial(A,T) = \{3, 4, 5\}$.



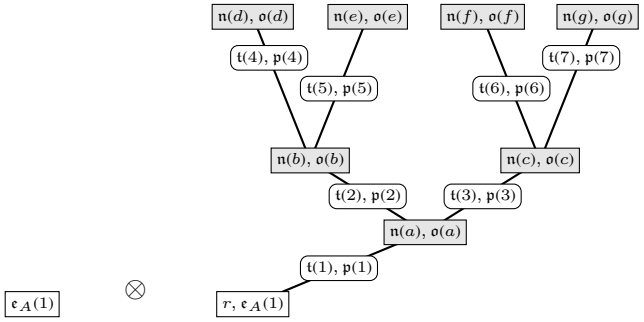
We suppose that $\mathfrak{t}(2) \in \mathfrak{L}_+$ but not $\mathfrak{t}(1)$. Then, we get:

$$\deg(4) = \deg(5) = 1 + \mathfrak{n}(a) + \mathfrak{n}(b), \quad \deg(3) = \mathfrak{n}(a).$$

We have for a fix $\mathfrak{e}_A : \partial(A,T) \to \mathbf{N}$:



where $\bar{r} = r - \mathfrak{n}(a) - \mathfrak{n}(b) - 1$. Now if A is just equal to the root of T, then one gets $N_A = \{\varrho\}$, $E_A = \emptyset$ and $\partial(A,T) = \{1\}$ as illustrated below



(2.18)

The map Δ^+ behaves the same way except that we start with a tree decorated by (r,m) at the root and that we exclude the case described in (2.18).

We use the symbolic notation to provide an alternative, recursive definition of the two maps $\Delta : \mathscr{H} \to \mathscr{H} \otimes \mathscr{H}_+$ and $\Delta^+ : \mathscr{H}_+ \to \mathscr{H}_+ \otimes \mathscr{H}_+$

$$\begin{aligned}
\Delta \mathbf{1} &= \mathbf{1} \otimes \mathbf{1}, \quad \Delta X^\ell = X^\ell \otimes \mathbf{1} \\
\Delta \mathcal{I}^r_{o_1}(X^\ell_k T) &= \Big(\mathcal{I}^r_{o_1}(X^\ell_k \cdot) \otimes \mathrm{id}\Big) \Delta \mathcal{D}_{r-\ell}(T) \\
\Delta \mathcal{I}^r_{o_2}(X^\ell_k T) &= \Big(\mathcal{I}^r_{o_2}(X^\ell_k \cdot) \otimes \mathrm{id}\Big) \Delta \mathcal{D}_{r-\ell-1}(T) + \sum_{m \le r+1} \frac{X^m}{m!} \otimes \mathcal{I}^{(r,m)}_{o_2}(X^\ell_k T) \\
\Delta^+ \mathcal{I}^{(r,m)}_{o_2}(X^\ell_k T) &= \Big(\mathcal{I}^{(r,m)}_{o_2}(X^\ell_k \cdot) \otimes \mathrm{id}\Big) \Delta \mathcal{D}_{r-\ell-1}(T) + \mathbf{1} \otimes \mathcal{I}^{(r,m)}_{o_2}(X^\ell_k T)
\end{aligned} \tag{2.19}$$

where $o_1 = (\mathfrak{t}_1, p_1)$, $\mathfrak{t}_1 \notin \mathfrak{L}_+$ and $o_2 = (\mathfrak{t}_2, p_2)$, $\mathfrak{t}_2 \in \mathfrak{L}_+$.

Remark 2.11 The maps Δ^+ and Δ are a variant of the maps used in [44, 12] for the recentering of iterated integrals in the context of singular SPDEs. They could be understood as a deformed Butcher-Connes-Kreimer coproduct. We present the ideas behind their construction:

- the decoration $\mathfrak{o}$ are inert and behave nicely toward the extraction/cutting operation.
- The recursive definition (2.19) is close to the definition of the Connes-Kreimer coproduct with the B_+ operator which grafts a forest onto a new root (see [30]).
- The deformation is given by the sum over m where root decorations are increased. This sum is finite bounded by $r+1$. This deformation corresponds to the one used for SPDEs but with a different projection. In Numerical Analysis, the length of the Taylor expansion is governed by the path connecting the root to the edge we are considering, whereas for SPDEs, it depends on the tree above the edge. Therefore, the structure proposed here is new in comparison to the literature and shows the universality of the deformation observed for singular SPDEs.
- There are some interesting simplifications in the definition of Δ and Δ^+ in comparison to [44, 12]. Indeed, one has

$$\Delta X^\ell = X^\ell \otimes \mathbf{1}$$

instead of the expected definition

$$\Delta X = X \otimes \mathbf{1} + \mathbf{1} \otimes X, \quad \Delta X^\ell = \sum_{m \leq \ell} \binom{\ell}{m} X^m \otimes X^{\ell-m}$$

and Δ^+ is not defined on polynomials. This comes from our numerical scheme: we are only interested in recentering around 0. Therefore, all the right part of the tensor product will be evaluated at zero and all these terms can be omitted at the level of the algebra. Such simplifications can also be used in the context of SPDEs. Indeed, if one considers random objects of the form $\Pi_x T$ which are recentered iterated integrals around the point x. When one wants to construct these stochastic objects, the interest lies in their law and it turns out that their law is invariant by translation. Then, one can only consider the term $\Pi_0 T$ which corresponds to the Numerical Analysis framework. With this simplification, we obtain an easier formulation for the antipode given in (2.30).

Remark 2.12 For the sequel, we will use mainly the symbolic notation (2.19) which is very useful for carrying out recursive proofs. We will also develop a recursive formulation of the general numerical scheme. This approach is also crucial in [44] and has been pushed forward in [10] for singular SPDEs.

In the next proposition, we prove the equivalence between the recursive and non-recursive definitions.

Proposition 2.13 *The definitions (2.16) and (2.17) coincide with (2.19).*

Proof. The operator Δ is multiplicative on $\hat{\mathscr{H}}$. It remains to verify that the recursive identities hold as well. We consider $\Delta\sigma$ with $\sigma = \mathcal{I}^r_{(\mathfrak{t}_2,p)}(X_k^\ell \tau)$ and $\mathfrak{t}_2 \in \mathfrak{L}_+$. We

write $\bar{\tau} = T^{\mathfrak{n},\mathfrak{o}}_{\mathfrak{e},r-\ell-1}$ and $\sigma = F^{\bar{\mathfrak{n}},\bar{\mathfrak{o}}}_{\bar{\mathfrak{e}},r}$ where

$$\bar{\mathfrak{e}} = \mathfrak{e} + \mathbf{1}_e(\mathfrak{t}_2, p), \quad \bar{\mathfrak{o}}(u) = \mathfrak{o} + \mathbf{1}_u k, \quad \bar{\mathfrak{n}}(u) = \mathfrak{n} + \mathbf{1}_u \ell$$

and e denotes a trunk of type $\mathfrak{t}$ created by $\mathcal{I}_{(\mathfrak{t}_2,p)}$, ϱ is the root of F and u is such that $e = (\varrho, u)$. It follows from these definitions that

$$\mathfrak{A}(F) = \{\{\varrho\}\} \cup \{A \cup \{\varrho, e\} \,:\, A \in \mathfrak{A}(T)\} \,.$$

Then, we have the identity

$$\begin{aligned}\Delta T &= (\mathcal{I}^r_{(\mathfrak{t}_2,p)}(X_k^\ell \cdot) \otimes \mathrm{id})\Delta\bar{\tau} + \sum_{\mathfrak{e}_A} \frac{1}{\mathfrak{e}_A!}(\bullet, \pi\mathfrak{e}_A, 0, 0, 0) \otimes (F, \mathfrak{n}, \mathfrak{o}, \mathfrak{e}, (r, \mathfrak{e}_A)) \\ &= \Big(\mathcal{I}^r_{(\mathfrak{t}_2,p)}(X_k^\ell \cdot) \otimes \mathrm{id}\Big)\Delta\mathcal{D}_{r-\ell-1}(\tau) + \sum_{m \le r+1} \frac{X^m}{m!} \otimes \mathcal{I}^{(r,m)}_{(\mathfrak{t}_2,p)}(X_k^\ell \tau)\end{aligned}$$

where the recursive $\Big(\mathcal{I}^r_{(\mathfrak{t}_2,p)}(X_k^\ell \cdot) \otimes \mathrm{id}\Big)\Delta$ encode the extraction of $A \cup \{\varrho, e\}$, $A \in \mathfrak{A}(T)$. We can perform a similar proof for $\mathfrak{t}_1 \notin \mathfrak{L}_+$ and for Δ^+. The main difference is that the sum on the polynomial decoration is removed for an edge not in $\mathfrak{L}_+$ and for Δ^+ such that we just keep the first term. □

Example 5 We illustrate the recursive definition of Δ by performing some computations on some relevant decorated trees that one can face in practice. For the decorated tree

$$T_1 = \mathcal{I}_{(\mathfrak{t}_2,0)}(X_k F_1) \quad F_1 = \mathcal{I}_{(\mathfrak{t}_1,1)}(X_{k_1})\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_2})\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_3})$$

which corresponds to the cubic Schrödinger equation, see Section A.1 in the appendix, we have that

$$\Delta\mathcal{D}_r(T_1) = \mathcal{D}_r(T_1) \otimes \mathbf{1} + \sum_{m \le r+1} \frac{X^m}{m!} \otimes \hat{\mathcal{D}}_{(r,m)}(T_1). \tag{2.20}$$

Relation (2.20) is proven as follows: Using the definition of $\mathcal{D}_r$ in (2.13) as well as (2.19) yields that

$$\begin{aligned}\Delta\mathcal{D}_r(T_1) &= \Delta\mathcal{I}^r_{(\mathfrak{t}_2,0)}(X_k F_1) \qquad (2.21)\\ &= \big(\mathcal{I}^r_{(\mathfrak{t}_2,0)}(X_k \cdot) \otimes \mathrm{id}\big)\Delta\mathcal{D}_{r-1}(F_1) + \sum_{m \le r+1} \frac{X^m}{m!} \otimes \mathcal{I}^{(r,m)}_{(\mathfrak{t}_2,0)}(X_k F_1).\end{aligned}$$

Thanks to the definition of $\hat{\mathcal{D}}_r$ in (2.14) we can conclude that

$$\mathcal{I}^{(r,m)}_{(\mathfrak{t}_2,0)}(X_k F_1) = \hat{\mathcal{D}}_{(r,m)}\mathcal{I}_{(\mathfrak{t}_2,0)}(X_k F_1) = \hat{\mathcal{D}}_{(r,m)}(T_1)$$

which yields together with (2.21) that

$$\Delta\mathcal{D}_r(T_1) = \big(\mathcal{I}^r_{(\mathfrak{t}_2,0)}(X_k \cdot) \otimes \mathrm{id}\big)\Delta\mathcal{D}_{r-1}(F_1) + \sum_{\ell \le r+1} \frac{X^\ell}{\ell!} \otimes \hat{\mathcal{D}}_{(r,\ell)}(T_1). \tag{2.22}$$

Next we need to analyse the term $\Big(\mathcal{I}^r_{(\mathfrak{t}_2,0)}(X_k\cdot)\otimes \mathrm{id}\Big)\Delta\mathcal{D}_{r-1}(F_1)$. First we use the multiplicativity of $\mathcal{D}_r$ (cf. (2.13)) and of the coproduct which yields that

$$\Delta\mathcal{D}_{r-1}(F_1) = \Big(\Delta\mathcal{I}^{r-1}_{(\mathfrak{t}_1,1)}(X_{k_1})\Big)\Big(\Delta\mathcal{I}^{r-1}_{(\mathfrak{t}_1,0)}(X_{k_2})\Big)\Big(\Delta\mathcal{I}^{r-1}_{(\mathfrak{t}_1,0)}(X_{k_3})\Big). \quad (2.23)$$

Thanks to (2.19) we furthermore have that

$$\begin{aligned}\Delta\mathcal{I}^{r-1}_{(\mathfrak{t}_1,p)}(X_{k_j}) &= \Big(\mathcal{I}^{r-1}_{(\mathfrak{t}_1,p)}(X_{k_j}\cdot)\otimes \mathrm{id}\Big)\Delta\mathcal{D}_{r-1}(\mathbf{1}) \\ &= \Big(\mathcal{I}^{r-1}_{(\mathfrak{t}_1,p)}(X_{k_j}\cdot)\otimes \mathrm{id}\Big)(\mathbf{1}\otimes\mathbf{1}) = \mathcal{I}^{r-1}_{(\mathfrak{t}_1,p)}(X_{k_j})\otimes\mathbf{1},\end{aligned} \quad (2.24)$$

where we have used that $\mathcal{D}_{r-1}(\mathbf{1}) = \mathbf{1}$ and $\Delta\mathbf{1} = \mathbf{1}\otimes\mathbf{1}$, see also (2.19). Plugging (2.24) into (2.23) yields that

$$\begin{aligned}&\Delta\mathcal{D}_{r-1}(F_1) \\ &\quad= \Big(\mathcal{I}^{r-1}_{(\mathfrak{t}_1,1)}(X_{k_1})\otimes\mathbf{1}\Big)\Big(\mathcal{I}^{r-1}_{(\mathfrak{t}_1,0)}(X_{k_2})\otimes\mathbf{1}\Big)\Big(\mathcal{I}^{r-1}_{(\mathfrak{t}_1,0)}(X_{k_3})\otimes\mathbf{1}\Big) \\ &\quad= \mathcal{I}^{r-1}_{(\mathfrak{t}_1,1)}(X_{k_1})\mathcal{I}^{r-1}_{(\mathfrak{t}_1,0)}(X_{k_2})\mathcal{I}^{r-1}_{(\mathfrak{t}_1,0)}(X_{k_3})\otimes\mathbf{1} = \mathcal{D}_{r-1}(F_1)\otimes\mathbf{1}.\end{aligned} \quad (2.25)$$

Hence,

$$\begin{aligned}\big(\mathcal{I}^r_{(\mathfrak{t}_2,0)}(X_k\cdot)\otimes\mathrm{id}\big)\Delta\mathcal{D}_{r-1}(F_1) &= \big(\mathcal{I}^r_{(\mathfrak{t}_2,0)}(X_k\cdot)\otimes\mathrm{id}\big)(\mathcal{D}_{r-1}(F_1)\otimes\mathbf{1}) \\ &= \mathcal{I}^r_{(\mathfrak{t}_2,0)}(X_kF_1)\otimes\mathbf{1} = \mathcal{D}_r(T_1)\otimes\mathbf{1}.\end{aligned}$$

Plugging this into (2.22) yields (2.20).

2.5 Hopf algbra and comodule structures

Using the two maps Δ and Δ^+, we want to identify a comodule structure over a Hopf algebra. Here, we provide a brief reminder of this structure for a reader not familiar with it. For simplicity, we will use the notation of the spaces introduced above as well as the maps Δ and Δ^+. The proof that we are indeed in this framework is then given in Proposition 2.15 below.

A *bialgebra* $(\mathcal{H}_+, \mathcal{M}, \mathbf{1}, \Delta^+, \mathbf{1}^\star)$ is given by:

- A vector space $\mathcal{H}_+$ over $\mathbf{C}$
- A linear map $\mathcal{M} : \mathcal{H}_+\otimes\mathcal{H}_+ \to \mathcal{H}_+$ (product) and an element $\eta : r \mapsto r\mathbf{1}$, $\mathbf{1}\in\mathcal{H}_+$ (identity) such that $(\mathcal{H}_+, \mathcal{M}, \eta)$ is a unital associative algebra.
- Linear maps $\Delta^+ : \mathcal{H}_+ \to \mathcal{H}_+\otimes\mathcal{H}_+$ (coproduct) and $\mathbf{1}^\star : \mathcal{H}_+ \to \mathbf{C}$ (counit), such that $(\mathcal{H}_+, \Delta^+, \mathbf{1}^\star)$ is a counital coassociative coalgebra, namely

$$(\Delta^+\otimes\mathrm{id})\Delta^+ = (\mathrm{id}\otimes\Delta^+)\Delta^+, \qquad (\mathbf{1}^\star\otimes\mathrm{id})\Delta^+ = (\mathrm{id}\otimes\mathbf{1}^\star)\Delta^+ = \mathrm{id} \quad (2.26)$$

- Δ^+ and $\mathbf{1}^*$ (resp. $\mathcal{M}$ and $\mathbf{1}$) are homomorphisms of algebras (coalgebras).

A *Hopf algebra* is a bialgebra $(\mathcal{H}_+, \mathcal{M}, \mathbf{1}, \Delta^+, \mathbf{1}^\star)$ endowed with a linear map $\mathcal{A} : \mathcal{H}_+ \to \mathcal{H}_+$ such that

$$\mathcal{M}(\mathrm{id}\otimes\mathcal{A})\Delta^+ = \mathcal{M}(\mathcal{A}\otimes\mathrm{id})\Delta^+ = \mathbf{1}^\star\mathbf{1}. \quad (2.27)$$

A *right comodule* over a bialgebra $(\mathscr{H}_+, \mathscr{M}, \mathbf{1}, \Delta^+, \mathbf{1}^\star)$ is a pair $(\mathscr{H}, \Delta)$ where $\mathscr{H}$ is a vector space and $\Delta : \mathscr{H} \to \mathscr{H} \otimes \mathscr{H}_+$ is a linear map such that

$$(\Delta \otimes \mathrm{id})\Delta = (\mathrm{id} \otimes \Delta^+)\Delta, \qquad (\mathrm{id} \otimes \mathbf{1}^\star)\Delta = \mathrm{id}. \tag{2.28}$$

In our framework, the product $\mathscr{M}$ is given by the forest product:

$$\mathscr{M}(T_1 \otimes T_2) = T_1 \cdot T_2.$$

Most of the properties listed above are quite straightforward to check. In the next proposition we focus on the coassociativity of the maps Δ and Δ^+ in (2.26) and (2.28).

Proposition 2.14 *One has:*

$$(\Delta \otimes \mathrm{id})\Delta = \big(\mathrm{id} \otimes \Delta^+\big)\Delta, \quad \big(\Delta^+ \otimes \mathrm{id}\big)\Delta^+ = \big(\mathrm{id} \otimes \Delta^+\big)\Delta^+.$$

Proof. We proceed by induction and we perform the proof only for $\mathscr{I}^r_{o_2}(X^\ell_k T)$. The other case follows similar steps. Note that

$$\begin{aligned}
&(\Delta \otimes \mathrm{id})\Delta \mathscr{I}^r_{o_2}(X^\ell_k T) \\
&= \Big(\Delta \mathscr{I}^r_{o_2}(X^\ell_k \cdot) \otimes \mathrm{id}\Big)\Delta \mathscr{D}_{r-\ell-1}(T) + \sum_{m \le r+1} \Delta \frac{X^m}{m!} \otimes \mathscr{I}^{(r,m)}_{o_2}(X^\ell_k T) \\
&= \sum_{m \le r+1} \frac{X^m}{m!} \otimes \Big(\mathscr{I}^{(r,m)}_{o_2}(X^\ell_k \cdot) \otimes \mathrm{id}\Big)\Delta \mathscr{D}_{r-\ell-1}(T) \\
&+ \sum_{m \le r+1} \frac{X^m}{m!} \otimes \mathbf{1} \otimes \mathscr{I}^{(r,m)}_{o_2}(X^\ell_k T) + \Big(\Big(\mathscr{I}^r_{o_2}(X^\ell_k \cdot) \otimes \mathrm{id}\Big)\Delta \otimes \mathrm{id}\Big)\Delta \mathscr{D}_{r-\ell-1}(T).
\end{aligned}$$

On the other hand, we get

$$\begin{aligned}
&\big(\mathrm{id} \otimes \Delta^+\big)\Delta \mathscr{I}^r_{o_2}(X^\ell_k T) \\
&= \Big(\mathscr{I}^r_{o_2}(X^\ell_k \cdot) \otimes \Delta^+\Big)\Delta \mathscr{D}_{r-\ell-1}(T) + \sum_{m \le r+1} \frac{X^m}{m!} \otimes \Delta^+ \mathscr{I}^{(r,m)}_{o_2}(X^\ell_k T) \\
&= \Big(\mathscr{I}^r_{o_2}(X^\ell_k \cdot) \otimes \Delta^+\Big)\Delta \mathscr{D}_{r-\ell-1}(T) + \sum_{m \le r+1} \frac{X^m}{m!} \otimes \mathbf{1} \otimes \mathscr{I}^{(r,m)}_{o_2}(X^\ell_k T) \\
&+ \sum_{m \le r+1} \frac{X^m}{m!} \otimes \Big(\mathscr{I}^{(r,m)}_{o_2}(X^\ell_k \cdot) \otimes \mathrm{id}\Big)\Delta \mathscr{D}_{r-\ell-1}(T).
\end{aligned}$$

Next we observe that

$$\begin{aligned}
\Big(\mathscr{I}^r_{o_2}(X^\ell_k \cdot) \otimes \Delta^+\Big)\Delta \mathscr{D}_{r-\ell-1}(T) &= \Big(\mathscr{I}^r_{o_2}(X^\ell_k \cdot) \otimes \mathrm{id} \otimes \mathrm{id}\Big)\big(\mathrm{id} \otimes \Delta^+\big)\Delta \mathscr{D}_{r-\ell-1}(T) \\
&= \Big(\mathscr{I}^r_{o_2}(X^\ell_k \cdot) \otimes \mathrm{id} \otimes \mathrm{id}\Big)(\Delta \otimes \mathrm{id})\Delta \mathscr{D}_{r-\ell-1}(T)
\end{aligned}$$

$$= \Big(\Big(\mathcal{I}^r_{o_2}(X^\ell_k \cdot) \otimes \mathrm{id}\Big)\Delta \otimes \mathrm{id}\Big)\Delta\mathcal{D}_{r-\ell-1}(T),$$

where we used an inductive argument for

$$(\Delta \otimes \mathrm{id})\Delta\mathcal{D}_{r-\ell-1}(T) = \big(\mathrm{id} \otimes \Delta^+\big)\Delta\mathcal{D}_{r-\ell-1}(T).$$

This yields the assertion. □

Proposition 2.15 *There exists an algebra morphism $\mathcal{A} : \mathcal{H}_+ \to \mathcal{H}_+$ so that $(\mathcal{H}_+, \cdot, \Delta^+, \mathbf{1}, \mathbf{1}^*, \mathcal{A})$ is a Hopf algebra. The map $\Delta : \mathcal{H} \to \mathcal{H} \otimes \mathcal{H}_+$ turns $\mathcal{H}$ into a right comodule for $\mathcal{H}_+$ with counit $\mathbf{1}^*$.*

Proof. From Proposition 2.14, $\mathcal{H}_+$ is a bialgebra and Δ is a coaction. In fact, $\mathcal{H}_+$ is a connected graded bialgebra with the grading given by the number of edges. Therefore, it is a Hopf algebra and we get the existence of a unique map called the antipode such that:

$$\mathcal{M}(\mathcal{A} \otimes \mathrm{id})\Delta^+ = \mathcal{M}(\mathrm{id} \otimes \mathcal{A})\Delta^+ = \mathbf{1}\mathbf{1}^*. \tag{2.29}$$

This concludes the proof. □

We use the identity (2.29) to write a recursive formulation for the antipode:

Proposition 2.16 *For every $T \in \hat{\mathcal{H}}$, one has*

$$\mathcal{A}\mathcal{I}^{(r,m)}_{o_2}(X^\ell_k T) = \mathcal{M}\Big(\mathcal{I}^{(r,m)}_{o_2}(X^\ell_k \cdot) \otimes \mathcal{A}\Big)\Delta\mathcal{D}_{r-\ell-1}(T). \tag{2.30}$$

Proof. We use the identity (2.29) which implies that

$$\mathcal{M}(\mathrm{id} \otimes \mathcal{A})\Delta^+\mathcal{I}^{(r,m)}_{o_2}(X^\ell_k T) = \mathbf{1}\,\mathbf{1}^*\Big(\mathcal{I}^{(r,m)}_{o_2}(X^\ell_k T)\Big).$$

As $\mathbf{1}^*$ is non-zero only on the empty forest we can thus conclude that

$$\mathcal{M}(\mathrm{id} \otimes \mathcal{A})\Delta^+\mathcal{I}^{(r,m)}_{o_2}(X^\ell_k T) = 0.$$

Then, we have by the definition of $\Delta^+\mathcal{I}^{(r,m)}_{o_2}(X^\ell_k T)$ given in (2.19) that

$$\mathcal{M}(\mathrm{id} \otimes \mathcal{A})\Big(\Big(\mathcal{I}^{(r,m)}_{o_2}(X^\ell_k \cdot) \otimes \mathrm{id}\Big)\Delta\mathcal{D}_{r-\ell-1}(T) + \mathbf{1} \otimes \mathcal{I}^{(r,m)}_{o_2}(X^\ell_k T)\Big) = 0$$

which yields (2.30). □

Remark 2.17 The formula (2.30) can be rewritten in a non-recursive form. Indeed, we introduced the reduced coproduct:

$$\tilde{\Delta}T = \Delta^+T - T \otimes \mathbf{1} - \mathbf{1} \otimes T.$$

Then, we can rewrite (2.29) as

$$\mathcal{A}T = -T - \sum_{(T)} T' \cdot (\mathcal{A}T'') \quad \tilde{\Delta}T = \sum_{(T)} T' \otimes T'',$$

where we have used Sweedler notations.

3 Approximating Iterated Integrals

3.1 A recursive formulation

For the rest of the section, an element of $\mathfrak{L}_+$ (resp, $\mathfrak{L}_+ \times \{0,1\}$) is denoted by $\mathfrak{t}_2$ (resp. o_2) and an element of $\mathfrak{L} \setminus \mathfrak{L}_+$ (resp. $\mathfrak{L} \setminus \mathfrak{L}_+ \times \{0,1\}$) is denoted by $\mathfrak{t}_1$ (resp. o_1). We denote by $\mathscr{C}$ the space of trigonometric polynomials which are functions of the form $z \mapsto \sum_j Q_j(z) e^{izP_j(k_1,\dots,k_n)}$ where the $Q_j(z)$ are polynomials in z and the P_j are polynomials in $k_1,\dots,k_n \in \mathbf{Z}^d$. The Q_j may also depend on $k_1,\dots,k_n$. We use the pointwise product on $\mathscr{C}$ for $F_1(z) = Q_1(z)e^{izP_1(k_1,\dots,k_n)}$ and $F_2(z) = Q_2(z)e^{izP_2(k_1,\dots,k_n)}$ given by:

$$(F_1F_2)(z) = Q_1(z)Q_2(z)e^{izP(k_1,\dots,k_n)}, \quad P = P_1 + P_2.$$

We want to define characters on decorated trees using their recursive construction. A character is a map defined from $\hat{\mathscr{H}}$ into $\mathscr{C}$ which respects the forest product. In the sense, that $g : \hat{\mathscr{H}} \to \mathscr{C}$ is a character if one has:

$$g(T \cdot \bar{T}) = g(T)g(\bar{T}), \quad T, \bar{T} \in \hat{\mathscr{H}}.$$

We define the following character $\Pi : \hat{\mathscr{H}} \to \mathscr{C}$ by

$$\begin{aligned} \Pi\big(T \cdot \bar{T}\big)(\tau) &= (\Pi T)(\tau)(\Pi \bar{T})(\tau) \\ \Pi\Big(\mathcal{I}_{o_1}(X_k^\ell T)\Big)(\tau) &= e^{i\tau P_{o_1}(k)}\tau^\ell(\Pi T)(\tau), \\ \Pi\Big(\mathcal{I}_{o_2}(X_k^\ell T)\Big)(\tau) &= -i|\nabla|^\alpha(k)\int_0^\tau e^{i\xi P_{o_2}(k)}\xi^\ell(\Pi T)(\xi)d\xi, \end{aligned} \tag{3.1}$$

where $T, \bar{T} \in \hat{\mathscr{H}}$.

We need a well chosen approximation of order r for the character Π defined in (3.1), which is suitable in the sense that it embeds those dominant frequencies matching the regularity n of the solution, see Remark 1.1. Therefore, we consider a new family of characters defined now on $\mathscr{H}$ and parametrised by $n \in \mathbf{N}$:

$$\begin{aligned} \Pi_n\big(T \cdot \bar{T}\big)(\tau) &= (\Pi_n T)(\tau)\big(\Pi_n \bar{T}\big)(\tau), \quad (\Pi_n X^\ell)(\tau) = \tau^\ell \\ (\Pi_n \mathcal{I}_{o_1}^r(X_k^\ell T))(\tau) &= \tau^\ell e^{i\tau P_{o_1}(k)}(\Pi_n \mathcal{D}_{r-\ell}(T))(\tau) \\ \Big(\Pi_n \mathcal{I}_{o_2}^r(X_k^\ell T)\Big)(\tau) &= \mathcal{K}_{o_2}^{k,r}\Big(\Pi_n\Big(X^\ell \mathcal{D}_{r-\ell-1}(T)\Big), n\Big)(\tau). \end{aligned} \tag{3.2}$$

All approximations are thereby carried out in the map $\mathcal{K}_{o_2}^{k,r}(\cdot, n)$ which is given in Definition 3.1 below. The main idea behind the map $\mathcal{K}_{o_2}^{k,r}(\cdot, n)$ is that all integrals are approximated through well-chosen Taylor expansions depending on the regularity n of the solution assumed a priori, and the interaction of the frequencies in the decorated trees. For a polynomial $P(k_1,\dots,k_n)$, we define the degree of P denoted by $\deg(P)$ as the maximum m such that k_i^m appears as a factor of one monomial in P for some i. For example:

$$\begin{aligned} P(k_1,k_2,k_3) &= -2k_1(k_2+k_3) + 2k_2k_3, \quad \deg(P) = 1 \\ P(k_1,k_2,k_3) &= k_1^2 - 2k_1(k_2+k_3) + 2k_2k_3, \quad \deg(P) = 2. \end{aligned}$$

Definition 3.1 Assume that $F : \xi \mapsto \xi^q e^{i\xi P(k_1,\dots,k_n)}$ where P is a polynomial in the frequencies $k_1, ..., k_n$ and let $o_2 = (\mathfrak{t}_2, p) \in \mathfrak{L}_+ \times \{0, 1\}$ and $r \in \mathbf{N}$. Let k be a linear map in $k_1, ..., k_n$ using coefficients in $\{-1, 0, 1\}$ and

$$\begin{aligned} \mathscr{L}_{\text{dom}} &= \mathscr{P}_{\text{dom}}(P_{o_2}(k) + P), \quad \mathscr{L}_{\text{low}} = \mathscr{P}_{\text{low}}(P_{o_2}(k) + P) \\ f(\xi) &= e^{i\xi\mathscr{L}_{\text{dom}}}, \quad g(\xi) = e^{i\xi\mathscr{L}_{\text{low}}}, \quad \bar{g}(\xi) = e^{i\xi\left(P_{o_2}(k)+P\right)}. \end{aligned}$$

Then, we define for $n \in \mathbf{N}$ and $r \geq q$

$$\mathscr{K}^{k,r}_{o_2}(F, n)(\tau) = \begin{cases} -i|\nabla|^\alpha(k) \displaystyle\sum_{\ell \leq r-q} \frac{\bar{g}^{(\ell)}(0)}{\ell!} \int_0^\tau \xi^{\ell+q} d\xi, \text{ if } n \geq \deg\left(\mathscr{L}^{r+1}_{\text{dom}}\right) + \alpha, \\ -i|\nabla|^\alpha(k) \displaystyle\sum_{\ell \leq r-q} \frac{g^{(\ell)}(0)}{\ell!} \Psi^r_{n,q}(\mathscr{L}_{\text{dom}}, \ell)(\tau), \quad \text{otherwise.} \end{cases} \tag{3.3}$$

Thereby we set for $(r - q - \ell + 1)\deg(\mathscr{L}_{\text{dom}}) + \ell \deg(\mathscr{L}_{\text{low}}) + \alpha > n$

$$\Psi^r_{n,q}(\mathscr{L}_{\text{dom}}, \ell)(\tau) = \int_0^\tau \xi^{\ell+q} f(\xi) d\xi. \tag{3.4}$$

Otherwise,

$$\Psi^r_{n,q}(\mathscr{L}_{\text{dom}}, \ell)(\tau) = \sum_{m \leq r-q-\ell} \frac{f^{(m)}(0)}{m!} \int_0^\tau \xi^{\ell+m+q} d\xi. \tag{3.5}$$

Here $\deg(\mathscr{L}_{\text{dom}})$ and $\deg(\mathscr{L}_{\text{low}})$ denote the degree of the polynomial $\mathscr{L}_{\text{dom}}$ and $\mathscr{L}_{\text{low}}$, respectively and $|\nabla|^\alpha(k) = \prod_{\alpha=\sum \gamma_j < \deg(\mathscr{L})} k_j^{\gamma_j}$ (cf. (1.6)). If $r < q$, the map $\mathscr{K}^{k,r}_{o_2}(F, n)(\tau)$ is equal to zero.

Remark 3.2 (Practical implementation) In practical computations we need to stabilise the above approach, as the Taylor series expansion of g may introduce derivatives on the numerical solution causing instability of the discretisation. We propose two ways to obtain stabilised high-order resonance based schemes without changing the underlying structure of the local error:

- Instead of straightforwardly applying a Taylor series expansion of g we introduce a stabilisation in the Taylor series expansion itself based on finite difference approximations of type $g'(0) = \frac{g(t)-g(0)}{t} + \mathcal{O}(tg'')$. For instance, at second- and third order we will use that

$$\begin{aligned} g(\xi) &= g(0) + \xi\frac{g(t) - g(0)}{t} + \mathcal{O}(t\xi g'') \\ g(\xi) &= g(0) + \xi\frac{g(t) + g(-t)}{\tau} + \frac{\xi^2}{2}\frac{g(t) - 2g(0) + g(-t)}{t^2} + \mathcal{O}(t\xi^2 g'''). \end{aligned} \tag{3.6}$$

  We refer to [36] for a simple recursive algorithm calculating the weights in compact finite difference formulas for any order of derivative and to any order of accuracy.

- We carry out a straightforward Taylor series expansion of g, but include suitable filter functions Ψ in the discretisation. At second-order they may for instance take the form

$$\Psi = \Psi(i\tau\mathscr{L}_{\text{low}}) \quad \text{with} \quad \Psi(0) = 1 \quad \text{and} \quad \left\|\tau\Psi(i\tau\mathscr{L}_{\text{low}})g'(0)\right\| \leq 1. \tag{3.7}$$

  For details on filter functions we refer to [43] and the references therein.

Practical computations and choices of this stabilisation for concrete examples are detailed in Appendix A.

Lemma 3.3 *We keep the notations of Definition 3.1. We suppose that $r \geq q$ then one has*

$$-i|\nabla|^{\alpha}(k)\int_0^{\tau}\xi^q f(\xi)g(\xi)d\xi - \mathscr{K}_{o_2}^{k,r}(F,n)(\tau) = \mathcal{O}(\tau^{r+2}k^{\bar{n}}) \tag{3.8}$$

where $\bar{n} = \max(n, \deg(\mathscr{L}_{low}^{r-q+1}) + \alpha)$.

Proof. It is just a consequence of Taylor expanding the functions $g, \bar{g}$ and f. If $n \geq \deg(\mathscr{L}_{\text{dom}}^r) + \alpha$ we have

$$\begin{aligned}
-i|\nabla|^{\alpha}(k)\int_0^{\tau}\xi^q f(\xi)g(\xi)d\xi + i|\nabla|^{\alpha}(k)\sum_{\ell\leq r-q}\frac{\bar{g}^{(\ell)}(0)}{\ell!}\int_0^{\tau}\xi^{\ell+q}d\xi \\
= \mathcal{O}(\tau^{r+2}|\nabla|^{\alpha}(k)\mathscr{L}_{\text{dom}}^{r+1}) \\
= \mathcal{O}(\tau^{r+2}k^{\bar{n}}).
\end{aligned}$$

Else, we get

$$\begin{aligned}
-i|\nabla|^{\alpha}(k)\int_0^{\tau}\xi^q f(\xi)g(\xi)d\xi + i|\nabla|^{\alpha}(k)\sum_{\ell\leq r-q}\frac{g^{(\ell)}(0)}{\ell!}\int_0^{\tau}\xi^{\ell+q}f(\xi)d\xi \\
= \mathcal{O}(\tau^{r+2}|\nabla|^{\alpha}(k)g^{(r-q+1)}) \\
= \mathcal{O}(\tau^{r+2}|\nabla|^{\alpha}(k)\mathscr{L}_{\text{low}}^{r-q+1})
\end{aligned}$$

where the latter follows from the observation that $g^{(\ell)}(\xi) = (i\mathscr{L}_{\text{low}})^{\ell}e^{i\xi\mathscr{L}_{\text{low}}}$.

If on the other hand $(r-q-\ell+1)\deg(\mathscr{L}_{\text{dom}}) + \ell\deg(\mathscr{L}_{\text{low}}) + \alpha \leq n$ then

$$\begin{aligned}
&-i|\nabla|^{\alpha}(k)\frac{g^{(\ell)}(0)}{\ell!}\int_0^{\tau}\xi^{\ell+q}f(\xi)d\xi + i|\nabla|^{\alpha}(k)\frac{g^{(\ell)}(0)}{\ell!}\sum_{m\leq r-q-\ell}\frac{f^{(m)}(0)}{m!}\int_0^{\tau}\xi^{\ell+m+q}d\xi \\
&= \frac{g^{(\ell)}(0)}{\ell!}\int_0^{\tau}\xi^{\ell+q}\mathcal{O}\left(\xi^{r-q-\ell+1}|\nabla|^{\alpha}(k)\mathscr{L}_{\text{dom}}^{r-q-\ell+1}\right)d\xi \\
&= \mathcal{O}(\tau^{r+2}|\nabla|^{\alpha}(k)\mathscr{L}_{\text{low}}^{\ell}\mathscr{L}_{\text{dom}}^{r-q-\ell+1}) \\
&= \mathcal{O}(\tau^{r+2}k^n)
\end{aligned}$$

which allows us to conclude. □

Remark 3.4 In the proof of Lemma 3.3, one has

$$\deg\left(\mathscr{L}_{\text{low}}^{\ell}\mathscr{L}_{\text{dom}}^{r-q-\ell+1}\right) \geq \deg\left(\mathscr{L}_{\text{low}}^{r-q+1}\right).$$

If $n = \deg\left(\mathscr{L}_{\text{low}}^{r-q+1}\right) + \alpha$ we cannot carry out a Taylor series expansion of f and we have to perform the integration exactly. This will give a more complicate numerical scheme. If on the other hand, n is larger, part of the Taylor expansions of f will be possible. In fact, n corresponds to the regularity of the solution we assume a priori, see Remark 1.1.

Remark 3.5 In Lemma 3.3 we express the approximation error in terms of powers of k. This will be enough for conducting the local error analysis for the general scheme. One can be more precise and keep the full structure by replacing k by monomials in $\mathscr{L}_{\text{dom}}$ and $\mathscr{L}_{\text{low}}$. This could be certainly useful when one wants to perform the global error analysis and needs to keep track of the full structure.

3.2 A Birkhoff type factorisation

The character $\Pi_n : \mathscr{H} \to \mathscr{C}$ is quite complex since one needs to compute several nonlinear interactions (oscillations) at the same time. Indeed, most of the time the operator $\mathscr{K}_{o_2}^{k,r}(\cdot, n)$ is applied to a linear combination of monomials of the form $e^{i\xi P_j(k)}$. We want to single out every oscillation through a factorisation of this character. We start by introducing a splitting with a projection $\mathbb{Q}$:

$$\mathscr{C} = \mathscr{C}_- \oplus \mathscr{C}_+, \quad \mathbb{Q} : \mathscr{C} \to \mathscr{C}_-$$

where $\mathscr{C}_-$ is the space of polynomials $Q(\xi)$ and $\mathscr{C}_+$ is the subspace of trigonometric polynomials which are elements of the form $z \mapsto \sum_j Q_j(z)e^{izP_j(k_1,\ldots,k_n)}$ with $P_j \neq 0$. Then we set

$$\mathscr{K}_{o_2,-}^{k,r} := \mathbb{Q} \circ \mathscr{K}_{o_2}^{k,r}, \quad \mathscr{K}_{o_2,+}^{k,r} := (\mathrm{id} - \mathbb{Q}) \circ \mathscr{K}_{o_2}^{k,r}. \tag{3.9}$$

One has

$$\mathscr{K}_{o_2}^{k,r} = \mathscr{K}_{o_2,-}^{k,r} + \mathscr{K}_{o_2,+}^{k,r}.$$

We define a character $A_n : \mathscr{H}_+ \to \mathbf{C}$ by

$$A_n(\mathscr{I}_{o_2}^{(r,m)}(X_k^{\ell}T)) = \Big(\mathbb{Q} \circ \partial^m \Pi_n \mathscr{I}_{o_2}^{r}(X_k^{\ell}T)\Big)(0). \tag{3.10}$$

The character A_n applied to $\mathscr{I}_{o_2}^{(r,m)}(X_k^{\ell}T)$ is extracting the coefficient of τ^m multiplied by $m!$ in $\Pi_n\mathscr{I}_{o_2}^{r}(X_k^{\ell}T)$. If we extend Π_n to $\mathscr{H}_+$ by setting

$$\Pi_n(\mathscr{I}_{o_2}^{(r,m)}(X_k^{\ell}T)) = \partial^m \Pi_n \mathscr{I}_{o_2}^{r}(X_k^{\ell}T)$$

then we have a new expression for A_n

$$A_n = (\mathbb{Q} \circ \Pi_n \cdot)(0). \tag{3.11}$$

We define a character $\hat{\Pi}_n : \mathscr{H} \to \mathscr{C}$ which computes only one interaction by applying repeatedly the projection $\mathrm{id} - \mathbb{Q}$.

$$\begin{aligned}\hat{\Pi}_n(\mathcal{I}^r_{o_1}(X^\ell_k T))(\tau) &= \tau^\ell e^{i\tau P_{o_1}(k)} \hat{\Pi}_n(\mathcal{D}_{r-\ell}(T))(\tau)\\ \hat{\Pi}_n(\mathcal{I}^r_{o_2}(X^\ell_k T)) &= \mathcal{K}^{k,r}_{o_2,+}(\hat{\Pi}_n(X^\ell \mathcal{D}_{r-\ell-1}(T)), n).\end{aligned} \tag{3.12}$$

We provide an identity for the approximation Π_n:

$$\Pi_n = \Big(\hat{\Pi}_n \otimes A_n\Big)\Delta. \tag{3.13}$$

Proposition 3.6 *The two definitions (3.2) and (3.13) coincide.*

Proof. We prove this identity by induction. We first consider a tree of the form $\mathcal{I}^r_{o_1}(X^\ell_k T)$ then we get:

$$\begin{aligned}\Big(\hat{\Pi}_n(\cdot)(\tau) \otimes A_n\Big)\Delta \mathcal{I}^r_{o_1}(X^\ell_k T) &= \Big(\hat{\Pi}_n\Big(\mathcal{I}^r_{o_1}(X^\ell_k \cdot)\Big)(\tau) \otimes A_n\Big)\Delta \mathcal{D}_{r-\ell}(T)\\ &= \tau^\ell e^{i\tau P_{o_1}(k)}\Big(\hat{\Pi}_n(\cdot)(\tau) \otimes A_n\Big)\Delta \mathcal{D}_{r-\ell}(T)\\ &= \tau^\ell e^{i\tau P_{o_1}(k)}(\Pi_n \mathcal{D}_{r-\ell}(T))(\tau)\\ &= \Big(\Pi_n \mathcal{I}^r_{o_1}(X^\ell_k T)\Big)(\tau),\end{aligned}$$

where we have used our inductive hypothesis. We look now at a tree of the form $\mathcal{I}^r_{o_2}(X^\ell_k T)$:

$$\begin{aligned}&\Big(\hat{\Pi}_n \otimes A_n\Big)\Delta \mathcal{I}^r_{o_2}(X^\ell_k T) = \Big(\hat{\Pi}_n(\mathcal{I}^r_{o_2}(X^\ell_k \cdot)) \otimes A_n\Big)\Delta \mathcal{D}_{r-\ell-1}(T)\\ &+ \sum_{m \le r+1} \frac{1}{m!}\hat{\Pi}_n(X^m) A_n(\mathcal{I}^{(r,m)}_{o_2}(X^\ell_k T))\\ &= \mathcal{K}^{r,k}_{o_2,+}\Big(\hat{\Pi}_n(X^\ell \cdot) \otimes A_n, n\Big)\Delta \mathcal{D}_{r-\ell-1}(T) + \mathcal{K}^{r,k}_{o_2,-}(\Pi_n X^\ell \mathcal{D}_{r-\ell-1}(T), n)\\ &= \mathcal{K}^{r,k}_{o_2,+}(\Pi_n X^\ell \mathcal{D}_{r-\ell-1}(T), n) + \mathcal{K}^{r,k}_{o_2,-}(\Pi_n X^\ell \mathcal{D}_{r-\ell-1}(T), n)\\ &= \Pi_n\Big(\mathcal{I}^r_{o_2}(X^\ell_k T)\Big)\end{aligned}$$

where we used the following identification

$$(\hat{\Pi}_n \otimes A_n)(T_1 \otimes T_2) = (\hat{\Pi}_n T_1 \otimes A_n T_2) = \hat{\Pi}_n(T_1) A_n(T_2)$$

and that

$$\begin{aligned}&\sum_{m \le r+1} \frac{1}{m!}\hat{\Pi}_n(X^m)\, A_n(\mathcal{I}^{(r,m)}_{o_2}(X^\ell_k T))\\ &= \sum_{m \le r+1} \frac{1}{m!}\hat{\Pi}_n(X^m)\Big(\mathbb{Q} \circ \partial^m \Pi_n \mathcal{I}^r_{o_2}(X^\ell_k T)\Big)(0)\\ &= \mathcal{K}^{r,k}_{o_2,-}(\Pi_n X^\ell \mathcal{D}_{r-1-\ell}(T), n).\end{aligned}$$

□

In the next proposition, we write a Birkhoff type factorisation for the character $\hat{\Pi}_n$ defined from Π_n and the antipode. Such an identity was also obtained in the context of SPDEs (see [12]) but with a twisted antipode. Our formulation is slightly simpler due to the simplifications observed at the level of the algebra (see Remark 2.11).

Proposition 3.7 *One has*

$$\hat{\Pi}_n = (\Pi_n \otimes (\mathbb{Q} \circ \Pi_n \mathscr{A} \cdot)(0))\Delta. \tag{3.14}$$

Proof. From (3.13), one gets:

$$\Pi_n = \Big(\hat{\Pi}_n \otimes (\mathbb{Q} \circ \Pi_n \cdot)(0)\Big)\Delta = \hat{\Pi}_n \star (\mathbb{Q} \circ \Pi_n \cdot)(0) \tag{3.15}$$

where the product $\star$ is defined from the coaction Δ. Then, if we multiply the identity (3.15) by the inverse $(\mathbb{Q} \circ \Pi_n \mathscr{A} \cdot)(0)$, we get

$$\begin{aligned}
\Pi_n \star (\mathbb{Q} \circ \Pi_n \mathscr{A} \cdot)(0) &= \Big(\hat{\Pi}_n \star (\mathbb{Q} \circ \Pi_n \cdot)(0)\Big) \star (\mathbb{Q} \circ \Pi_n \mathscr{A} \cdot)(0) \\
&= \Big(\Big(\hat{\Pi}_n \otimes (\mathbb{Q} \circ \Pi_n \cdot)(0)\Big)\Delta \otimes (\mathbb{Q} \circ \Pi_n \mathscr{A} \cdot)(0)\Big)\Delta \\
&= \Big(\hat{\Pi}_n \otimes ((\mathbb{Q} \circ \Pi_n \cdot)(0) \otimes (\mathbb{Q} \circ \Pi_n \mathscr{A} \cdot)(0))\Delta^+\Big)\Delta \\
&= \hat{\Pi}_n
\end{aligned}$$

where we have used

$$(\Delta \otimes \mathrm{id})\Delta = \big(\mathrm{id} \otimes \Delta^+\big)\Delta, \quad \mathscr{M}(\mathrm{id} \otimes \mathscr{A})\Delta^+ = \mathbf{1}^*.$$

This concludes the proof. □

3.3 Local error analysis

In this section, we explore the properties of the character $\hat{\Pi}_n$ which allows us to conduct the local error analysis of the approximation given by Π_n. Proposition 3.8 below shows that only one oscillation is treated through $\hat{\Pi}_n$.

Proposition 3.8 *For every forest $T \in \hat{\mathscr{H}}$, there exists a polynomial $B_n(\mathscr{D}_r(T))$ such that*

$$\hat{\Pi}_n(\mathscr{D}_r(T))(\xi) = B_n(\mathscr{D}_r(T))(\xi) e^{i\xi \mathscr{R}_{dom}(T)}$$

where $\mathscr{R}_{dom}(T)$ is given in Definition 2.5. Moreover, $B_n(\mathscr{D}_r(T))(\xi)$ is given by:

$$B_n(\mathscr{D}_r(T))(\xi) = \frac{P(\xi)}{Q}, \quad Q = \prod_{\bar{T} \in A} \big(\mathscr{R}_{dom}(\bar{T})\big)^{m_{\bar{T}}} \tag{3.16}$$

where $P(\xi)$ is a polynomial in ξ and the k_i, A is a set of decorated subtrees of T satisfying the same property as in Corollary 2.9.

Proof. We proceed by induction. We get

$$\begin{aligned}\hat{\Pi}_n\big(\mathcal{D}_r(T\cdot\bar{T})\big)(\xi) &= \hat{\Pi}_n(\mathcal{D}_r(T))(\xi)\hat{\Pi}_n\big(\mathcal{D}_r(\bar{T})\big)(\xi)\\ &= B_n(\mathcal{D}_r(T))(\xi)e^{i\xi\mathcal{R}_{\text{dom}}(T)}B_n\big(\mathcal{D}_r(\bar{T})\big)(\xi)e^{i\xi\mathcal{R}_{\text{dom}}(\bar{T})}\\ &= B_n(\mathcal{D}_r(T))(\xi)\hat{B}_n\big(\mathcal{D}_r(\bar{T})\big)(\xi)e^{i\xi(\mathcal{R}_{\text{dom}}(\bar{T})+\mathcal{R}_{\text{dom}}(\bar{T}))}\\ &= B_n\big(\mathcal{D}_r(T\cdot\bar{T})\big)(\xi)e^{i\xi\mathcal{R}_{\text{dom}}(T\cdot\bar{T})}.\end{aligned}$$

The pointwise product preserves the structure given by (3.16).

Then for $T=\mathcal{I}_{o_1}(X_k^\ell\bar{T})$, one gets by the definition of $\hat{\Pi}_n$ given in (3.12) that

$$\begin{aligned}\hat{\Pi}_n(\mathcal{D}_r(T))(\xi) &= \xi^\ell e^{i\xi P_{o_1}(k)}\hat{\Pi}_n\big(\mathcal{D}_{r-\ell}(\bar{T})\big)(\xi)\\ &= \xi^\ell e^{i\xi P_{o_1}(k)+i\xi\mathcal{R}_{\text{dom}}(\bar{T})}\hat{\Pi}_n\big(\mathcal{D}_{r-\ell}(\bar{T})\big)(\xi)\\ &= B_n(\mathcal{D}_r(T))(\xi)e^{i\xi\mathcal{R}_{\text{dom}}(T)}.\end{aligned}$$

One gets $B_n(\mathcal{D}_r(T))(\xi)=\xi^\ell B_n\big(\mathcal{D}_r(\bar{T})\big)(\xi)$ and can conclude on the preservation of the factorisation (3.16). We end with the decorated tree $T=\mathcal{I}_{o_2}(X_k^\ell\bar{T})$. By the definition of $\hat{\Pi}_n$ given in (3.12) we obtain that

$$\hat{\Pi}_n(T)(\xi)=\mathcal{K}^{k,r}_{o_2,+}(\hat{\Pi}_n(X^\ell\mathcal{D}_{r-\ell-1}(\bar{T})),n)(\xi).$$

Now, we apply the induction hypothesis on $\bar{T}$ which yields

$$\hat{\Pi}_n(\mathcal{D}_{r-\ell-1}(\bar{T}))(\xi)=B_n(\mathcal{D}_{r-\ell-1}(\bar{T}))(\xi)e^{i\xi\mathcal{R}_{\text{dom}}(\bar{T})}$$

and we conclude by applying Definition 3.1. Indeed, by applying $\mathcal{K}^{k,r}_{o_2,+}$ to $\xi^\ell e^{i\xi\mathcal{R}_{\text{dom}}(\bar{T})}$, we can get in (3.4) extras terms $\frac{1}{Q}$ coming from expressions of the form

$$\int_0^\tau \xi^{\ell+q}e^{i\xi\mathcal{R}_{\text{dom}}(T)}d\xi.$$

Then, by computing this integral, we obtain coefficients of the form

$$\frac{1}{(i\mathcal{R}_{\text{dom}}(T))^{m_T}}$$

if $\mathcal{R}_{\text{dom}}(T))^{m_T}\neq 0$. This term will be multiplied by $B_n(\mathcal{D}_{r-\ell-1}(\bar{T}))(\xi)e^{i\xi\mathcal{R}_{\text{dom}}(\bar{T})}$ and preserves the structure given in (3.16). When performing the Taylor series expansions by applying $\mathcal{K}^{k,r}_{o_2,+}$ (cf. (3.3) and (3.5)) we can also get some extra polynomials in the k_i. This leads to the factor $P(\xi)$ in (3.16) and concludes the proof. □

The next recursive definition introduces a systematic way to compute the local error from the structure of the decorated tree and the coaction Δ.

Definition 3.9 Let $n \in \mathbf{N}$, $r \in \mathbf{Z}$. We recursively define $\mathscr{L}^r_{\text{low}}(\cdot, n)$ as

$$\mathscr{L}^r_{\text{low}}(T, n) = 1, \quad r < 0.$$

Else

$$\begin{aligned} \mathscr{L}^r_{\text{low}}(\mathbf{1}, n) = 1, \quad \mathscr{L}^r_{\text{low}}(T \cdot \bar{T}, n) &= \mathscr{L}^r_{\text{low}}(T, n) + \mathscr{L}^r_{\text{low}}(\bar{T}, n) \\ \mathscr{L}^r_{\text{low}}(\mathcal{I}_{o_1}(X^\ell_k T), n) &= \mathscr{L}^{r-\ell}_{\text{low}}(T, n) \\ \mathscr{L}^r_{\text{low}}(\mathcal{I}_{o_2}(X^\ell_k T), n) &= \mathscr{L}^{r-\ell-1}_{\text{low}}(T, n) + \mathbf{1}_{\{r-\ell \geq 0\}} \sum_j k^{\bar{n}_j} \end{aligned}$$

where

$$\begin{aligned} \sum_j T_j = \mathscr{M}_{(1)} \Delta \mathscr{D}_{r-\ell-1}(T), \quad T_j \in H, \quad \mathscr{M}_{(1)}(T_1 \otimes T_2) = T_1, \\ \bar{n}_j = \max(n, \deg(\mathscr{R}_{\text{low}}(\mathcal{I}_{(\mathfrak{t}_2, p)}(X^\ell_k T_j))^{r-\ell+1} + \alpha), \end{aligned}$$

and $\mathscr{R}_{\text{low}}$ is defined in Definition 2.5.

Remark 3.10 As in Remark 3.5, we use only powers of k in Definition 3.9 but more structures can be preserved if one wants to conduct a global error analysis.

Now we are in the position to state the approximation error of Π^r_n to Π (cf. (1.19)).

Theorem 3.11 *For every $T \in \mathcal{T}$ one has,*

$$(\Pi T - \Pi^r_n T)(\tau) = \mathcal{O}\big(\tau^{r+2} \mathscr{L}^r_{low}(T, n)\big)$$

where Π is defined in (3.1), Π_n is given in (3.2) and $\Pi^r_n = \Pi_n \mathscr{D}_r$.

Proof. We proceed by induction by using the recursive definition (3.2) of Π_n.

First, one gets:

$$(\Pi - \Pi^r_n)(\mathbf{1})(\tau) = 0 = \mathcal{O}\big(\tau^{r+2} \mathscr{L}^r_{\text{low}}(\mathbf{1}, n)\big).$$

One also has

$$\begin{aligned} (\Pi - \Pi^r_n)(\mathcal{I}_{o_1}(X^\ell_k T))(\tau) &= \tau^\ell e^{i\tau P_{o_1}(k)} (\Pi - \Pi^{r-\ell}_n)(T)(\tau) \\ &= \mathcal{O}\Big(\tau^{r+2} \mathscr{L}^{r-\ell}_{\text{low}}(T, n)\Big). \end{aligned}$$

Then, one gets again by (3.1) and (3.2) that

$$\begin{aligned} (\Pi - \Pi^r_n)(T \cdot \bar{T})(\tau) &= (\Pi - \Pi^r_n)(T)(\tau)(\Pi^r_n \bar{T})(\tau) + (\Pi T)(\tau)(\Pi - \Pi^r_n)(\bar{T})(\tau) \\ &= \mathcal{O}\big(\tau^{r+2} \mathscr{L}^r_{\text{low}}(T, n)\big) + \mathcal{O}\big(\tau^{r+2} \mathscr{L}^r_{\text{low}}(\bar{T}, n)\big) \\ &= \mathcal{O}\big(\tau^{r+2} \mathscr{L}^r_{\text{low}}(T \cdot \bar{T}, n)\big) \end{aligned}$$

where we use Definition 3.9. At the end, by (3.1) and (3.2) and inserting zero in terms of

$$\pm\Pi_n^{r-\ell-1}(T)(\xi)$$

as well as using that $\Pi_n^{r-\ell-1}(T) = \Pi_n \mathcal{D}_{r-\ell-1}(T)$ we obtain

$$\begin{aligned}
&(\Pi - \Pi_n^r)\Big(\mathcal{I}_{o_2}(X_k^\ell T)\Big)(\tau) = -i|\nabla|^\alpha(k)\int_0^\tau \xi^\ell e^{i\xi P_{o_2}(k)}(\Pi - \Pi_n^{r-\ell-1})(T)(\xi)d\xi \\
&- i|\nabla|^\alpha(k)\int_0^\tau e^{i\xi P_{o_2}(k)}(\Pi_n X^\ell \mathcal{D}_{r-\ell-1}(T))(\xi)d\xi - \mathcal{K}_{o_2}^{k,r}(\Pi_n(X^\ell \mathcal{D}_{r-\ell-1}(T)), n)(\tau) \\
&= \int_0^\tau \mathcal{O}\Big(\xi^{r+1}\mathcal{L}_{\text{low}}^{r-\ell-1}(T,n)\Big)d\xi + \mathbf{1}_{\{r-\ell\geq 1\}}\sum_j \mathcal{O}(\tau^{r+2}k^{\bar{n}_j}) \\
&= \mathcal{O}\big(\tau^{r+2}\mathcal{L}_{\text{low}}^r(T,n)\big)
\end{aligned}$$

where

$$\sum_j T_j = \mathcal{M}_{(1)}\Delta T, \quad \mathcal{M}_{(1)}(T_1 \otimes T_2) = T_1.$$

$$\bar{n}_j = \max(n, \deg(\mathcal{R}_{\text{low}}(\mathcal{I}_{o_2}(X_k^\ell T_j)))^{r-\ell+1}) + \alpha).$$

Note that in the above calculation we have used the following decomposition

$$\Pi_n(\mathcal{D}_{r-\ell-1}(T)) = \Big(\hat{\Pi}_n \otimes A_n\Big)\Delta\mathcal{D}_{r-\ell-1}(T)$$

which by Proposition 3.8 implies that there exist $a_j \in \mathbf{C}$ such that

$$\Pi_n(\mathcal{D}_{r-\ell-1}(T))(\xi) = \sum_j a_j B_n(\mathcal{D}_{r-\ell-1}(T_j))(\xi)e^{i\xi\mathcal{R}_{\text{dom}(T_j)}},$$

where $B_n(\mathcal{D}_{r-\ell-1}(T_j))(\xi) = b_j + \mathcal{O}(\xi)$ for some constant b_j.

Thus by applying Lemma 3.3 with $F = \sum_j b_j e^{i\xi\mathcal{R}_{\text{dom}(T_j)}} + \mathcal{O}(\xi)$, we get an error for every term in the sum which is at most of the form:

$$\mathcal{O}(\tau^{r+2}k^{\bar{n}_j}).$$

This concludes the proof.

□

Proposition 3.12 *For every decorated tree $T = \mathcal{I}_{(\mathfrak{t},p)}^r(X_k^\ell \bar{T})$ in $\mathcal{T}$, one can map $\Pi_n T$ back into Physical space which means that for functions indexed by the leaves of T, $(v_u)_{u\in L_T}$, the term*

$$\mathcal{F}^{-1}\left(\sum_{k=\sum_{u\in L_T} a_u k_u} (\Pi_n T)(\xi)\right)(v_{u,a_u}, u \in L_T) \tag{3.17}$$

can be expressed by applying classical differential operators $\nabla^\ell, e^{i\xi\nabla^m}$, $m, \ell \in \mathbf{Z}$ to v_{u,a_u} which are defined by $v_{u,1} = v_u$ and $v_{u,-1} = \overline{v_u}$.

Proof. We proceed by induction using the identity (3.13). The latter implies that

$$\Pi_n T = \Big(\hat{\Pi}_n \otimes A_n\Big)\Delta T = \sum_j \hat{\Pi}_n(T_j^{(1)})A_n(T_j^{(2)}) \quad \Delta T = \sum_j T_j^{(1)} \otimes T_j^{(2)}.$$

Then, for every $\hat{\Pi}_n T_j^{(1)}$, we apply Proposition 3.8 and we get:

$$\hat{\Pi}_n\Big(T_j^{(1)}\Big)(\xi) = B_n\Big(T_j^{(1)}\Big)(\xi)e^{i\xi\mathscr{R}_{\text{dom}}(T_j^{(1)})}.$$

Moreover, $B_n(T_j^{(1)})(\xi)$ is given by:

$$B_n(\mathscr{D}_r(T_j^{(1)}))(\xi) = \frac{P(\xi)}{Q}, \quad Q = \prod_{\bar{T}\in A(T_1^{(j)})} \big(\mathscr{R}_{\text{dom}}(\bar{T})\big)^{m_{\bar{T}}} \tag{3.18}$$

with the notations defined in Proposition 3.8 and $A(T_j^{(1)})$ are some decorated subtrees of $T_j^{(1)}$. The term $\hat{\Pi}_n\Big(T_j^{(1)}\Big)(\xi)$ can be mapped back to Physical space using Proposition 2.4. The polynomial $P(\xi)$ will produce derivatives of type ∇^ℓ and the term $e^{i\xi\mathscr{R}_{\text{dom}}(T_j^{(1)})}$ is of the form $e^{i\xi\nabla^m}$. For the terms $A_n(T_j^{(2)})$, we use the non-recursive definition of the map Δ. Indeed, $T_j^{(2)}$ is a product of trees of the form T_e where e is an edge in T which was cut. The map A_n is defined from Π_n in (3.10). Then we can apply the induction hypothesis on $A_n(T_e)$. For each $T_e = \mathscr{I}_{(\mathfrak{t},p)}(X_{k_e}^{\ell_e}\bar{T}_e)$, k_e appears as a decoration at a leaf of $T_j^{(1)}$. Then, it is either included in Q or disjoint. This allows us to apply the inverse Fourier Transform concluding the proof. □

4 A general numerical scheme

Recall the mild solution of (1.1) given by Duhamel's formula

$$u(t) = e^{it\mathscr{L}(\nabla,\frac{1}{\varepsilon})}v - i|\nabla|^\alpha e^{it\mathscr{L}(\nabla,\frac{1}{\varepsilon})}\int_0^t e^{-i\xi\mathscr{L}(\nabla,\frac{1}{\varepsilon})}p(u(t),\bar{u}(t))d\xi. \tag{4.1}$$

For simplicity we restrict our attention to nonlinearities of type

$$p(u,\bar{u}) = u^N\bar{u}^M \tag{4.2}$$

which includes all examples in Appendix A. The analysis which follows can straightforwardly be generalised to polynomials and coupled systems.

In order to describe our general numerical scheme, we first describe the iterated integrals produced by the (high order) iteration of Duhamel's formula (4.1) through a class of suitable decorated trees.

4.1 Decorated trees generated by Duhamel's formula

With the aid of the Fourier series expansion $u(x) = \sum_{k\in\mathbf{Z}^d} \hat{u}_k(t)e^{ikx}$ we first rewrite Duhamel's formula (4.1) at the level of the Fourier coefficients:

$$\hat{u}_k(t) = e^{itP(k)}\hat{v}_k - i|\nabla|^\alpha(k)e^{itP(k)}\int_0^t e^{-i\xi P(k)}p_k(u(\xi),\bar{u}(\xi))d\xi \tag{4.3}$$

where $P(k)$ denotes the differential operator $\mathscr{L}$ in Fourier space, i.e.,

$$P(k) = \mathscr{L}\left(\nabla, \frac{1}{\varepsilon}\right)(k)$$

(cf. (1.6) and (1.7), respectively) and

$$p_k(u(t),\bar{u}(t)) = \sum_{k=\sum_i k_i - \sum_j \bar{k}_j} \prod_{i=1}^N \hat{u}_{k_i}(t) \prod_{j=1}^M \bar{\hat{u}}_{\bar{k}_j}(t).$$

This equation is given in an abstract way by

$$U_k = \mathcal{I}_{(\mathfrak{t}_1,0)}(X_k) + \mathcal{I}_{(\mathfrak{t}_1,0)}(X_k\mathcal{I}_{(\mathfrak{t}_2,0)}(X_k p_k(U,\bar{U}))) \tag{4.4}$$

where

$$p_k(U,\bar{U}) = \sum_{k=\sum_i k_i - \sum_j \bar{k}_j} \prod_{i=1}^N U_{k_i} \prod_{j=1}^M \bar{U}_{\bar{k}_j}$$

and $\mathfrak{L} = \{\mathfrak{t}_1, \mathfrak{t}_2\}$, $P_{\mathfrak{t}_1}(X) = P(X)$ and $P_{\mathfrak{t}_2}(X) = -P(X)$.

Remark 4.1 The two systems (4.3) and (4.4) are equivalent. Indeed, we can define a map ψ such that:

$$\begin{aligned}
\psi(U_k)(u,v,t) &= \hat{u}_k(t), \quad \psi(\bar{U}_k)(u,v,t) = \bar{\hat{u}}_k(t)\\
\psi(\mathcal{I}_{o_1}(X_k))(v,u,t) &= e^{itP_{o_1}(k)}\hat{v}_k(t)\\
\psi(\mathcal{I}_{o_1}(X_kT))(v,u,t) &= e^{itP_{o_1}(k)}\psi(T)(v,u,t)\\
\psi(\mathcal{I}_{o_2}(X_kT))(v,u,t) &= -i|\nabla|^\alpha(k)\int_0^t e^{i\xi P_{o_2}(k)}\psi(T)(v,u,\xi)d\xi.
\end{aligned}$$

In this notation (4.3) takes the form

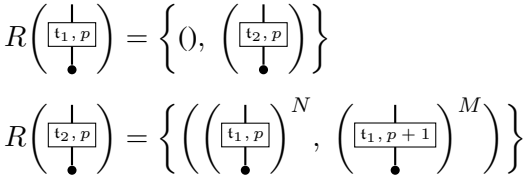
$$\psi(U_k) = \psi(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k))(v,u,0) + \psi\big(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k\mathcal{I}_{(\mathfrak{t}_2,1)}(X_k p_k(U,\bar{U})))\big).$$

We define the notion of a rule in the same spirit as in [12]. A rule is then a map R assigning to each element of $\mathfrak{L}\times\{0,1\}$ a non-empty collection of tuples in $\mathfrak{L}\times\{0,1\}$. The relevant rule describing the class of equations (4.4) is given by

$$R((\mathfrak{t}_1,p)) = \{(),((\mathfrak{t}_2,p))\}$$

$$R((\mathfrak{t}_2, p)) = \{((\mathfrak{t}_1, p)^N, (\mathfrak{t}_1, p+1)^M)\}$$

where N and M depend on the polynomial nonlinearity (4.2) and the notation $(\mathfrak{t}_1, p+1)^M$ means that $(\mathfrak{t}_1, p+1)$ is repeated M times and the sum $p+1$ is performed modulo 2. Using graphical notation, one gets:



(4.5)

Definition 4.2 A decorated tree $T_{\mathfrak{e}}^{\mathfrak{o}}$ in $\hat{\mathcal{T}}_0$ is generated by R if for every node u in N_T, one has

$$\cup_{e \in E_u} (\mathfrak{t}(e), \mathfrak{p}(e)) \in R(e_u)$$

where $E_u \subset E_T$ are the edges of the form (u, v) and e_u is the edge of the form (w, u). The set of decorated trees generated by R is denoted by $\hat{\mathcal{T}}_0(R)$ and for $r \in \mathbf{Z}$, $r \geq -1$, we set:

$$\hat{\mathcal{T}}_0^r(R) = \{T_{\mathfrak{e}}^{\mathfrak{o}} \in \hat{\mathcal{T}}_0 \,, \deg(T_{\mathfrak{e}}^{\mathfrak{o}}) \leq r+1\}.$$

Given a decorated tree $T_{\mathfrak{e}} = (T, \mathfrak{e})$ where we just have the edge decoration, the symmetry factor $S(T_{\mathfrak{e}})$ is defined inductively by setting $S(\mathbf{1}) = 1$, while if T is of the form

$$\prod_{i,j} \mathcal{I}_{(\mathfrak{t}_{t_i}, p_i)}(T_{i,j})^{\beta_{i,j}}$$

with $T_{i,j} \neq T_{i,\ell}$ for $j \neq \ell$, then

$$S(T) = \Big(\prod_{i,j} S(T_{i,j})^{\beta_{i,j}} \beta_{i,j}! \Big) \,. \tag{4.6}$$

We extend this definition to any tree $T_{\mathfrak{e}}^{\mathfrak{n},\mathfrak{o}}$ in $\mathcal{T}$ by setting:

$$S(T_{\mathfrak{e}}^{\mathfrak{n},\mathfrak{o}}) := S(T_{\mathfrak{e}}).$$

Then, we define the map $\Upsilon^p(T)(v)$ for

$$T = \mathcal{I}_{(\mathfrak{t}_2,0)}(X_k \prod_{i=1}^{N} \mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_i} T_i) \prod_{j=1}^{M} \mathcal{I}_{(\mathfrak{t}_1,1)}(X_{\tilde{k}_j} \tilde{T}_j))$$

by

$$\Upsilon^p(T)(v) = \partial_v^N \partial_{\bar{v}}^M p(v, \bar{v}) \prod_{i=1}^{N} \Upsilon^p(X_{k_i} T_i)(v) \prod_{j=1}^{M} \overline{\Upsilon^p(X_{\tilde{k}_j} \tilde{T}_j)(v)} \tag{4.7}$$

$$= N!M! \prod_{i=1}^{N} \Upsilon^p(X_{k_i} T_i)(v) \prod_{j=1}^{M} \overline{\Upsilon^p(X_{\tilde{k}_j} \tilde{T}_j)(v)}.$$

and

$$\Upsilon^p(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k))(v) = \hat{v}_k, \quad \Upsilon^p(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k\tilde{T}))(v) = \Upsilon^p(X_k\tilde{T})(v),$$
$$\Upsilon^p(\mathcal{I}_{(\mathfrak{t}_1,1)}(X_k))(v) = \bar{\hat{v}}_k, \quad \Upsilon^p(\mathcal{I}_{(\mathfrak{t}_1,1)}(X_k\tilde{T}))(v) = \overline{\Upsilon^p(X_k\tilde{T})(v)}, \quad \tilde{T} \neq \mathbf{1}.$$

Example 6 Assume that we have the tree

$$T = \mathcal{I}_{(\mathfrak{t}_2,0)}(X_k \mathcal{I}_{(\mathfrak{t}_1,1)}(X_{k_1}) \mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_2}) \mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_3}))$$

then

$$\begin{aligned}\Upsilon^p(T)(v) &= 2\Upsilon^p(\mathcal{I}_{(\mathfrak{t}_1,1)}(X_{k_1}))(v)\Upsilon^p(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_2}))(v)\Upsilon^p(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_3}))(v)\\ &= 2\bar{\hat{v}}_{k_1}\hat{v}_{k_2}\hat{v}_{k_3}\end{aligned}$$

and $S(T) = 2$.

If we want to find a solution U to (4.4) as a linear combination of decorated trees, then we need to give a meaning to the conjugate of U that is $\bar{U}$. We define this operation on $\hat{\mathcal{T}}$ recursively as:

$$\overline{\mathcal{I}_{(\mathfrak{t},p)}(X_k T)} = \mathcal{I}_{(\mathfrak{t},p+1)}(X_k \overline{T}), \quad \overline{T_1 \cdot T_2} = \overline{T}_1 \cdot \overline{T}_2. \tag{4.8}$$

This map is well-defined from $\hat{\mathcal{H}}$ into itself and preserves the identity (2.1). We want to find maps V_k^r, $r \in \mathbf{Z}$, $r \geq -1$ such that

$$V_k^{r+1} = \mathcal{I}_{(\mathfrak{t}_1,0)}(X_k) + \mathcal{I}_{(\mathfrak{t}_1,0)}(X_k \mathcal{I}_{(\mathfrak{t}_2,0)}(X_k p_k(V^r, \overline{V^r}))). \tag{4.9}$$

An explicit expression is given in the next proposition

Proposition 4.3 *The solution in $\hat{\mathcal{H}}$ of (4.9) is given by the trees generated by the rule R*

$$V_k^r(v) = \sum_{T \in \hat{\mathcal{T}}_0^r(R)} \frac{\Upsilon^p(X_k T)(v)}{S(T)} \mathcal{I}_{(\mathfrak{t}_1,0)}(X_k T).$$

Proof. We will prove this by induction. We need to expand

$$Z_k = \mathcal{I}_{(\mathfrak{t}_1,0)}(X_k) + \mathcal{I}_{(\mathfrak{t}_1,0)}(X_k \mathcal{I}_{(\mathfrak{t}_2,0)}(X_k p_k(V^r, \overline{V^r}))). \tag{4.10}$$

One has

$$Z_k = \mathcal{I}_{(\mathfrak{t}_1,0)}(X_k) + \sum_{T_i, \tilde{T}_j \in \hat{\mathcal{T}}_0^r(R)} \sum_{k = \sum_i k_i - \sum_j \tilde{k}_j} \prod_{i,j} \frac{\Upsilon^p(T_i)}{S(T_i)} \frac{\overline{\Upsilon^p(\tilde{T}_j)}}{S(\tilde{T}_j)}$$

$$\cdot \mathcal{I}_{(\mathfrak{t}_1,0)}(X_k \mathcal{I}_{(\mathfrak{t}_2,0)}(X_k \left(\prod_i \mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_i} T_i) \prod_j \mathcal{I}_{(\mathfrak{t}_1,1)}(X_{\tilde{k}_j} \tilde{T}_j) \right))).$$

Then, we fix the products $\prod_i \mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_i} T_i)$ and $\prod_j \mathcal{I}_{(\mathfrak{t}_1,0)}(X_{\tilde{k}_j} \tilde{T}_j)$ which can be rewritten as follows

$$\prod_i \mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_i} T_i) = \prod_\ell \mathcal{I}_{(\mathfrak{t}_1,0)}(X_{m_\ell} F_\ell)^{\beta_\ell}$$
$$\prod_j \mathcal{I}_{(\mathfrak{t}_1,1)}(X_{\tilde{k}_j} \tilde{T}_j) = \prod_\ell \mathcal{I}_{(\mathfrak{t}_1,1)}(X_{\tilde{m}_\ell} \tilde{F}_\ell)^{\alpha_\ell}$$

where the F_ℓ (resp. $\tilde{F}_\ell$) are disjoints. The number of times the same term appears when we sum over the F_ℓ (resp. $\tilde{F}_\ell$) and the k_i (resp. $\tilde{k}_j$) is equal to $\frac{N!}{\prod_\ell \beta_\ell!}$ (resp. $\frac{M!}{\prod_\ell \alpha_\ell!}$). With the identity

$$\prod_{i,j} \frac{\Upsilon^p(T_i)}{S(T_i)} \frac{\overline{\Upsilon^p(\tilde{T}_j)}}{S(\tilde{T}_j)} \frac{N!}{\prod_\ell \beta_\ell!} \frac{M!}{\prod_\ell \alpha_\ell!} = \frac{\Upsilon^p(X_k T)}{S(T)}$$

we thus get

$$Z_k = \sum_{T \in \hat{\mathcal{T}}_0^{r+1}(R)} \frac{\Upsilon^p(X_k T)}{S(T)} \mathcal{I}_{(\mathfrak{t}_1,0)}(X_k T) = V_k^{r+1}$$

which concludes the proof. □

Before describing our numerical scheme, we need to remove the trees which are already of size $\mathcal{O}(\tau^{r+2})$. Indeed, one has

$$(\Pi T)(\tau) = \mathcal{O}(\tau^{n_+(T)})$$

where $n_+(T)$ is the number of edges of type in $\mathfrak{L}_+$ corresponding to the number of integration in the definition of ΠT. Therefore, we define the space of trees $\mathcal{T}_0^r(R)$ as

$$\mathcal{T}_0^r(R) = \{T \in \hat{\mathcal{T}}_0^r(R),\ n_+(T) \leq r+1\}. \tag{4.11}$$

4.2 Numerical scheme and local error analysis

Now, we are able to describe the general numerical scheme:

Definition 4.4 (The general numerical scheme) For fixed $n, r \in \mathbf{N}$, we define the general numerical scheme in Fourier space as:

$$U_k^{n,r}(\tau, v) = \sum_{T \in \mathcal{T}_0^{r+2}(R)} \frac{\Upsilon^p(X_k T)(v)}{S(T)} \Pi_n(\mathcal{D}_r(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k T)))(\tau). \tag{4.12}$$

Remark 4.5 We can always map the term $U_k^{n,r}(\tau, v)$ back to physical using classical operators. Indeed, from Proposition 3.12 this holds true for each term $\Pi_n(\mathcal{D}_r(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k T)))(\tau)$. In practical applications this will allow us to carry out the multiplication of functions in physical space, using the Fast Fourier Transform (cf. Remark 1.3). Details for concrete applications are given in Appendix A.

Remark 4.6 The spaces $\mathcal{V}_k^r$ given in (1.17) and (1.18) are defined by:

$$\mathcal{V}_k^r = \{\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k T),\, T \in \mathcal{T}_0^{r+2}(R)\}.$$

The numerical scheme (4.12) approximates the exact solution locally up to order $r+2$. More precisely, the following Theorem holds,

Theorem 4.7 (Local error) *The numerical scheme (4.12) with initial value $v = u(0)$ approximates the exact solution $U_k(\tau, v)$ up to a local error of type*

$$U_k^{n,r}(\tau, v) - U_k(\tau, v) = \sum_{T \in \mathcal{T}_0^{r+2}(R)} \mathcal{O}\big(\tau^{r+2} \mathcal{L}_{low}^r(T, n) \Upsilon^p(X_k T)(v)\big)$$

where the operator $\mathcal{L}_{low}^r(T, n)$, given in Definition 3.9, embeds the necessary regularity of the solution.

Proof. First we define the exact solution u^r up to order r in Fourier space by

$$U_k^r(\tau, v) = \sum_{T \in \mathcal{T}_0^{r+2}(R)} \frac{\Upsilon^p(X_k T)(v)}{S(T)} \Pi(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k T))(\tau)$$

which satisfies

$$u(\tau) - u^r(\tau) = \mathcal{O}\big(\tau^{r+2} |\nabla|^{\alpha(r+2)} \tilde{p}(u(t))\big) \tag{4.13}$$

for some polynomial $\tilde{p}$ and $0 \le t \le \tau$. Thanks to Proposition 3.11 we furthermore obtain that

$$\begin{aligned} &U_k^{n,r}(\tau, v) - U_k^r(\tau, v) \qquad (4.14)\\ &\quad = \sum_{T \in \mathcal{T}_0^{r+2}(R)} \frac{\Upsilon^p(X_k T)}{S(T)}(v)(\Pi - \Pi_n^r)(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k T))(\tau) \\ &\quad = \sum_{T \in \mathcal{T}_0^{r+2}(R)} \mathcal{O}\big(\tau^{r+2} \mathcal{L}_{\text{low}}^r(T, n) \Upsilon^p(X_k T)(v)\big). \end{aligned}$$

Next we write

$$U_k^{n,r}(\tau, v) - U_k(\tau, v) = U_k^{n,r}(\tau, v) - U_k^r(\tau, v) + U_k^r(\tau, v) - U_k(\tau, v)$$

where by the definition of $\mathcal{L}_{\text{low}}^r(T, n)$ we easily see that the approximation error (4.14) is dominant compared to (4.13). □

Remark 4.8 Theorem 4.7 allows us to state the order of consistency of the general scheme (4.12) as well as the necessary regularity requirements on the exact solution to meet the error bound (note that $\mathscr{L}^r_{\text{low}}(T,n)$ could be ∞). In Appendix A we detail the particular form of the general scheme (4.12) on concrete examples and explicitly determine the required regularity of the solution in the local error imposed by the operator $\mathscr{L}^r_{\text{low}}(T,n)$.

Remark 4.9 Theorem 4.7 provides a local error estimate (order of consistency) for the new resonance based schemes (4.12). With the aid of stability one can easily obtain a global error estimate with the aid of Lady Windamere's fan argument [43]. However, the necessary stability estimates in general rely on the algebraic structure of the underlying space. In the stability analysis of dispersive PDEs set in Sobolev spaces H^r one classically exploits bilinear estimates of type

$$\|vw\|_r \leq c_{r,d}\|v\|_r\|w\|_r.$$

The latter only hold for $r > d/2$ and thus restricts the analysis to sufficiently smooth Sobolev spaces H^r with $r > d/2$. To obtain (sharp) L^2 global error estimates one needs to exploit discrete Strichartz estimates and discrete Bourgain spaces in the periodic setting, see, e.g., [52, 68]. This is out of the scope of this paper.

Proposition 4.10 *For n sufficiently large the scheme (4.12) coincides with a classical numerical discretisation based on Taylor series expansions of the full operator $\mathscr{L}$.*

Proof. From Theorem 4.7, one has

$$U_k^{n,r}(\tau,v) - U_k^r(\tau,v) = \sum_{T\in\mathscr{T}_0^{r+2}(R)} \mathcal{O}\big(\tau^{r+2}\mathscr{L}^r_{\text{low}}(T,n)\Upsilon^p(X_kT)(v)\big).$$

We need to show that for n bigger than $\deg(P^r_{t_2})$, $U_k^{n,r}(\tau,v)$ is a polynomial in τ and that $\mathscr{L}^r_{\text{low}}(T,n) = \mathcal{O}(P^r_{t_2}(k))$. Then by mapping it back to the physical space, we get:

$$U^{n,r}(\tau,v) - U^r(\tau,v) = \mathcal{O}(\tau^{r+2}\partial_t^r v)$$

where $U^{n,r}(\tau,v)$ is a polynomial in τ. The two statements can be proven by induction. One needs to see how these properties are preserved by applying the map $\mathscr{K}^{k,r}_{o_2}(\cdot,n)$. Indeed, one has

$$\Big(\Pi_n\mathscr{I}^r_{o_2}(X_k^\ell T)\Big)(\tau) = \mathscr{K}^{k,r}_{o_2}\Big(\Pi_n\Big(X^\ell\mathscr{D}_{r-\ell-1}(T)\Big),n\Big)(\tau).$$

Then by the induction hypothesis, we can assume that $\Pi_n\big(X^\ell\mathscr{D}_{r-\ell-1}(T)\big)(\xi)$ is a polynomial in ξ where the coefficients are polynomials in k. Then by applying Definition 3.1, one has:

$$\bar{g}(\xi) = e^{i\xi P_{o_2}(k)}.$$

One can see that if $n \geq \deg(P^r_{t_2})$ then one Taylor expands $\bar{g}$ which yields a polynomial in τ with polynomial coefficients in k. Lemma 3.3 implies an error of order $\mathcal{O}(k^n)$. This concludes the proof. □

Remark 4.11 Proposition 4.10 implies that we indeed recover classical numerical discretisations with our general framework for smooth solutions. More precisely, one could check that depending on the particular choice of filter functions Ψ (cf. Remark 3.2) we recover exponential Runge–Kutta methods and exponential integrators, respectively. For details on the latter we refer to [7, 18, 46] and the references therein.

Appendix A Applications

We illustrate the general framework presented in Section 4 on three concrete examples. First we consider the nonlinear Schrödinger and the Korteweg-de Vries equation, for which we find a new class of second-order resonance based schemes. For an extensive overview on classical, non-resonance based discretisations we thereby refer to [8, 20, 21, 29, 33, 35, 37, 46, 48, 49, 50, 51, 52, 55, 58, 62, 73, 74] and the references therein. In addition, we illustrate the general framework on a highly oscillatory system: the Klein–Gordon equation in the so-called non-relativistic limit regime, where the speed of light formally tends to infinity, see, e.g., [1, 2, 3, 4, 5, 25].

A.1 Nonlinear Schrödinger

We consider the cubic nonlinear Schrödinger equation

$$i\partial_t u + \Delta u = |u|^2 u \tag{A.1}$$

with mild solution given by Duhamel's formula

$$u(\tau) = e^{i\tau\Delta}u(0) - ie^{i\tau\Delta}\int_0^\tau e^{-i\xi\Delta}\big(|u(\xi)|^2 u(\xi)\big)d\xi. \tag{A.2}$$

The Schrödinger equation (A.1) fits into the general framework (1.1) with

$$\mathcal{L}\left(\nabla, \frac{1}{\varepsilon}\right) = \Delta, \quad \alpha = 0 \quad \text{and} \quad p(u,\overline{u}) = u^2\overline{u}.$$

Here $\mathcal{L} = \{\mathfrak{t}_1, \mathfrak{t}_2\}$, $P_{\mathfrak{t}_1} = -X^2$ and $P_{\mathfrak{t}_2} = X^2$ (cf (2.4)). Then, we denoted by $\mathbf{|}$ an edge decorated by $(\mathfrak{t}_1, 0)$, $\vdots$ an edge denoted by $(\mathfrak{t}_1, 1)$ by $|$ an edge decorated by $(\mathfrak{t}_2, 0)$ and by $\vdots$ an edge decorated by $(\mathfrak{t}_2, 1)$. The rules that generate the trees obtained by iterating Duhamel's formulation are given by:

$$R(|) = R(\vdots) = \{(\mathbf{|}, \mathbf{|}, \vdots)\}\,, \quad R(\mathbf{|}) = \{(|), ()\}\,, \quad R(\vdots) = \{(|), ()\}\,.$$

A.1.1 First-order schemes

The general framework (4.12) derived in Section 4 builds the foundation of the first-order resonance based schemes presented below for the nonlinear Schrödinger equation (A.1). The structure of the schemes depends on the regularity of the solution.

Corollary A.1 *For the nonlinear Schrödinger equation (A.1) the general scheme (4.12) takes at first order the form*

$$u^{\ell+1} = e^{i\tau\Delta}u^\ell - i\tau e^{i\tau\Delta}\Big((u^\ell)^2\varphi_1(-2i\tau\Delta)\overline{u^\ell}\Big) \tag{A.3}$$

with a local error of order $\mathcal{O}(\tau^2|\nabla|u)$ *and filter function* $\varphi_1(\sigma) = \frac{e^\sigma - 1}{\sigma}$.

In case of regular solutions the general scheme (4.12) takes the simplified form

$$u^{\ell+1} = e^{i\tau\Delta}u^\ell - i\tau e^{i\tau\Delta}\Big(|u^\ell|^2u^\ell\Big) \tag{A.4}$$

with a local error of order $\mathcal{O}(\tau^2\Delta u)$.

Remark A.2 With the general framework introduced in Section 4 we exactly recover the first-order resonance based low regularity scheme (A.3) proposed in [67]. In addition, for smooth solution we recover a classical first-order approximation (A.4), i.e., the exponential Euler method, with a classical local error $\mathcal{O}\big(\tau^2\Delta u\big)$. The low regularity scheme (A.3) allows us to solve a larger class of solution due to its favorable error behavior at low regularity.

Above we used a simplified notation: Let φ^τ and Φ^τ denote the exact and numerical solution at time $t = \tau$, i.e., $\varphi^\tau(v) = u(\tau)$ and $\Phi^\tau(v) = u^1 \approx u(\tau)$. We write

$$\varphi^\tau(v) - \Phi^\tau(v) = \mathcal{O}_{\|\cdot\|}\Big(\tau^\gamma\tilde{\mathscr{L}}v\Big) \tag{A.5}$$

if in a suitable norm $\|\cdot\|$ (e.g., Sobolev norm) it holds that

$$\|\varphi^\tau(v) - \Phi^\tau(v)\| \le C(T,d,r)\tau^\gamma \sup_{0\le t\le\tau}\|q\Big(\tilde{\mathscr{L}}\varphi^t(v)\Big)\|$$

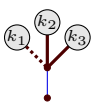
for some polynomial q, differential operator $\tilde{\mathscr{L}}$ and constant C independent of τ. If (A.5) holds we say that the numerical solution u^1 approximates the exact solution $u(t)$ at time $t = \tau$ with a local error of order $\mathcal{O}\Big(\tau^\gamma\tilde{\mathscr{L}}v\Big)$.

Proof. **Construction of the schemes.** For the first-order scheme we need a local error of order $\mathcal{O}(\tau^2)$. Therefore, we need to choose $r = 0$ in Definition 4.4 and the corresponding trees accordingly. From Definition (4.4), the scheme is given by

$$U_k^{n,0}(\tau,v) = \sum_{T\in\mathcal{T}_0^2(R)}\frac{\Upsilon^p(X_kT)(v)}{S(T)}\Pi_n(\mathscr{D}_0(\mathscr{I}_{(\mathfrak{t}_1,0)}(X_kT)))(\tau) \tag{A.6}$$

where one has

$$\mathcal{T}_0^2(R) = \{T_0, T_1,\, k_i \in \mathbf{Z}^d\}, \quad T_0 = \mathbf{1} \quad \text{and} \quad T_1 = \quad$$



with T_1 associated to the first order iterated integral

$$\mathcal{I}_1(v^2, \overline{v}, \xi) = \int_0^\xi e^{-i\xi_1\Delta}\left[\left(e^{i\xi_1\Delta}v\right)^2\left(e^{-i\xi_1\Delta}\overline{v}\right)\right]d\xi_1. \tag{A.7}$$

Hence, our first-order scheme (A.6) takes the form

$$\begin{aligned} U_k^{n,0}(\tau, v) = &\frac{\Upsilon^p(X_k)(v)}{S(\mathbf{1})}\Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k)))(\tau) \\ &+ \sum_{\substack{k_1,k_2,k_3\in\mathbf{Z}^d \\ -k_1+k_2+k_3=k}} \frac{\Upsilon^p(X_kT_1)(v)}{S(T_1)}\Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_1)))(\tau). \end{aligned} \tag{A.8}$$

In order to write down the scheme (A.8) explicitly, we need to compute

$$\begin{aligned} &\Upsilon^p(X_k)(v), \quad S(\mathbf{1}) \quad \text{and} \quad \Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k)))(\tau) \\ &\Upsilon^p(X_kT_1)(v), \quad S(T_1) \quad \text{and} \quad \Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_1)))(\tau). \end{aligned}$$

Note that if we use the symbolic notation, one gets:

$$T_1 = \mathcal{I}_{(\mathfrak{t}_2,0)}(X_kF_1) \quad F_1 = \mathcal{I}_{(\mathfrak{t}_1,1)}(X_{k_1})\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_2})\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_3}), \quad k = -k_1 + k_2 + k_3. \tag{A.9}$$

Thanks to the definition of Υ^p, S and Example 6 we already know that

$$\Upsilon^p(X_k)(v) = \hat{v}_k, \quad S(\mathbf{1}) = 1, \quad \Upsilon^p(X_kT_1)(v) = 2\overline{\hat{v}}_{k_1}\hat{v}_{k_2}\hat{v}_{k_3}, \quad S(T) = 2.$$

Hence, the scheme (A.8) takes the form

$$\begin{aligned} U_k^{n,0}(\tau, v) = &\hat{v}_k\Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k)))(\tau) \\ &+ \sum_{\substack{k_1,k_2,k_3\in\mathbf{Z}^d \\ -k_1+k_2+k_3=k}} \overline{\hat{v}}_{k_1}\hat{v}_{k_2}\hat{v}_{k_3}\Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_1)))(\tau). \end{aligned} \tag{A.10}$$

It remains to compute $\Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_j)))(\tau)$ for $j = 0, 1$ with $T_0 = \mathbf{1}$ and T_1 given in (A.9).

1. Computation of $\Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k)))(\tau)$. The second line in (3.2) together with $P_{\mathfrak{t}_1}(k) = -k^2$ implies that

$$\Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k)))(\tau) = \Pi_n(\mathcal{I}^0_{(\mathfrak{t}_1,0)}(X_k))(\tau) = e^{i\tau P_{\mathfrak{t}_1}(k)} = e^{-i\tau k^2}.$$

2. Computation of $\Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_1)))(\tau)$. The definition of the tree T_1 in (A.9) furthermore implies that

$$\begin{aligned} \Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_1)))(\tau) &= (\Pi_n\mathcal{I}^0_{(\mathfrak{t}_1,0)}(X_kT_1))(\tau) = e^{i\tau P_{\mathfrak{t}_1}(k)}(\Pi_n\mathcal{D}_0(T_1))(\tau) \\ &= e^{-i\tau k^2}(\Pi_n\mathcal{I}^0_{(\mathfrak{t}_2,0)}(X_kF_1))(\tau). \end{aligned} \tag{A.11}$$

Furthermore, by the third line in (3.2) we have

$$\big(\Pi_n \mathcal{I}^0_{(\mathfrak{t}_2,0)}(X_k F_1)\big)(\tau) = \mathcal{K}^{k,0}_{(\mathfrak{t}_2,0)}(\Pi_n \mathcal{D}_{-1}(F_1), n)(\tau)$$

By the multiplicativity of Π_n (see (3.2)) we furthermore obtain

$$\begin{aligned}\Pi_n \mathcal{D}_{-1}(F_1)(\xi) &= \Big(\Pi_n \mathcal{I}^{-1}_{(\mathfrak{t}_1,1)}(X_{k_1})\Big)(\xi)\Big(\Pi_n \mathcal{I}^{-1}_{(\mathfrak{t}_1,0)}(X_{k_2})\Big)(\xi)\Big(\Pi_n \mathcal{I}^{-1}_{(\mathfrak{t}_1,0)}(X_{k_3})\Big)(\xi)\\ &= e^{(-1)i\xi P_{\mathfrak{t}_1}(-k_1)}(\Pi_n \mathbf{1})(\xi) e^{i\xi P_{\mathfrak{t}_1}(k_2)}(\Pi_n \mathbf{1})(\xi) e^{i\xi P_{\mathfrak{t}_1}(k_3)}(\Pi_n \mathbf{1})(\xi)\\ &= e^{i\xi(k_1^2 - k_2^2 - k_3^2)}\end{aligned}$$

where we used again that $P_{\mathfrak{t}_1}(k_j) = -k_j^2$. Collecting the results and plugging them into (A.11) yields that

$$(\Pi_n \mathcal{I}^0_{(\mathfrak{t}_1,0)}(X_k T_1))(\tau) = e^{-i\tau k^2} \mathcal{K}^{k,0}_{(\mathfrak{t}_2,0)}\Big(e^{i\xi(k_1^2 - k_2^2 - k_3^2)}, n\Big)(\tau). \tag{A.12}$$

Next we use Definition 3.1. Observe that (see Example 4),

$$\begin{aligned}&\mathcal{L}_{\text{dom}} = 2k_1^2, \quad \mathcal{L}_{\text{low}} = -2k_1(k_2 + k_3) + 2k_2 k_3\\ &f(\xi) = e^{i\xi \mathcal{L}_{\text{dom}}}, \quad g(\xi) = e^{i\xi \mathcal{L}_{\text{low}}}\end{aligned} \tag{A.13}$$

and thus as $g(0) = 1$ we have

$$\mathcal{K}^{k,0}_{(\mathfrak{t}_2,0)}\Big(e^{i\xi(k_1^2 - k_2^2 - k_3^2)}, n\Big)(\tau) = \begin{cases} -i\tau, & \text{if } n \geq 2\\ -i\Psi^0_{n,0}(\mathcal{L}_{\text{dom}}, 0)(\tau), & \text{if } n < 2\end{cases}$$

with

$$\Psi^0_{n,0}(\mathcal{L}_{\text{dom}}, 0)(\tau) = \int_0^\tau f(\xi) d\xi = \frac{e^{2i\tau k_1^2} - 1}{2ik_1^2} = \tau \varphi_1(2i\tau k_1^2), \quad \text{if } n < 2. \tag{A.14}$$

Plugging this into (A.12) yields together with (A.11) and (A.10) that

$$\begin{aligned}U_k^{n=1,0}(\tau, v) &= e^{-i\tau k^2}\hat{v}_k - i\tau \sum_{\substack{k_1,k_2,k_3 \in \mathbf{Z}^d\\ -k_1+k_2+k_3=k}} \overline{\hat{v}}_{k_1} \hat{v}_{k_2} \hat{v}_{k_3} e^{-i\tau k^2} \varphi_1(2i\tau k_1^2)\\ U_k^{n>1,0}(\tau, v) &= e^{-i\tau k^2}\hat{v}_k - i\tau \sum_{\substack{k_1,k_2,k_3 \in \mathbf{Z}^d\\ -k_1+k_2+k_3=k}} \overline{\hat{v}}_{k_1} \hat{v}_{k_2} \hat{v}_{k_3} e^{-i\tau k^2}.\end{aligned} \tag{A.15}$$

Note that the above Fourier based resonance schemes can easily be transformed back to physical space yielding the two first-order iterative schemes (A.3) and (A.4) which depend on the smoothness n of the exact solution.

Local error analysis. It remains to show that the general local error bound stated in Theorem 4.7 implies the local error estimates

$$\mathcal{O}\big(\tau^2 \nabla^n\big), \quad n = 1, 2 \tag{A.16}$$

for the schemes (A.3) (with $n = 1$) and (A.4) (with $n = 2$), respectively. Theorem 4.7 implies that

$$U_k^{n,0}(\tau, v) - U_k^0(\tau, v) = \sum_{T \in \mathcal{T}_0^2(R)} \mathcal{O}\big(\tau^2 \mathcal{L}_{\text{low}}^0(T, n) \Upsilon^p(X_k T)(v)\big)$$

By Definition 3.9 we have that $\mathcal{L}_{\text{low}}^0(T_0) = 1$ and

$$\mathcal{L}_{\text{low}}^0(T_1) = \mathcal{L}_{\text{low}}^0(\mathcal{I}_{(\mathfrak{t}_2,0)}(X_k F_1), n) = \mathcal{L}_{\text{low}}^{-1}(F_1, n) + \sum_j k^{\overline{n}_j}$$

$$\overline{n}_j = \max(n, \deg(\mathcal{R}_{\text{low}}(\mathcal{I}_{(\mathfrak{t}_2,0)}(X_k^\ell F_j))))$$

where $\sum_j F_j = \mathcal{M}_{(1)} \Delta F_1$ with $\mathcal{M}_{(1)}(F_1 \otimes F_2) = F_1$. Note that by (2.25) we have that $\Delta F_1 = F_1 \otimes \mathbf{1}$ such that $\sum_j F_j = F_1$. Hence,

$$\overline{n}_j = \overline{n}_1 = \max(n, \deg(\mathcal{R}_{\text{low}}(\mathcal{I}_{(\mathfrak{t}_2,0)}(X_k F_1)))).$$

By Definition 2.5 and Example 4 we obtain that

$$\mathcal{R}_{\text{low}}(\mathcal{I}_{(\mathfrak{t}_2,0)}(X_k F_1) = -2k_1(k_2 + k_3) + 2k_2 k_3.$$

Hence, $\overline{n}_1 = \max(n, 1)$ and

$$\begin{aligned}
\mathcal{L}_{\text{low}}^0(T_1) &= \mathcal{L}_{\text{low}}^{-1}(F_1, n) + k^{\max(n,1)} \\
&= \mathcal{L}_{\text{low}}^{-1}(\mathcal{I}_{(\mathfrak{t}_1,1)}(X_{k_1}), n) + \mathcal{L}_{\text{low}}^{-1}(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_2}), n) \\
&\quad + \mathcal{L}_{\text{low}}^{-1}(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_3}), n) + k^{\max(n,1)} \\
&= \mathcal{L}_{\text{low}}^{-1}(\mathbf{1}, n) + \mathcal{L}_{\text{low}}^{-1}(\mathbf{1}, n) + \mathcal{L}_{\text{low}}^{-1}(\mathbf{1}, n) + k^{\max(n,1)}.
\end{aligned}$$

Using that $\mathcal{L}_{\text{low}}^{-1}(\mathbf{1}, n) = 1$ we finally obtain that $\mathcal{L}_{\text{low}}^0(T_1) = \mathcal{O}(k^{\max(n,1)})$. Therefore, we recover (A.16). □

A.1.2 Second-order approximation

The general framework (4.12) derived in Section 4 builds the foundation of the second-order resonance based schemes presented below for the nonlinear Schrödinger equation (A.1). The structure of the schemes depends on the regularity of the solution.

Corollary A.3 *For the nonlinear Schrödinger equation (A.1) the general scheme (4.12) takes at second order the form*

$$\begin{aligned}
u^{\ell+1} = e^{i\tau\Delta} u^\ell - i\tau e^{i\tau\Delta}\Big((u^\ell)^2(\varphi_1(-2i\tau\Delta) - \varphi_2(-2i\tau\Delta))\overline{u^\ell} \\
+ \Big(e^{i\tau\Delta} u^\ell\Big)^2 \varphi_2(-2i\tau\Delta) e^{i\tau\Delta}\overline{u^\ell}\Big) - \frac{\tau^2}{2} e^{i\tau\Delta}\Big(|u^\ell|^4 u^\ell\Big)
\end{aligned} \tag{A.17}$$

with a local error of order $\mathcal{O}(\tau^3 \Delta u)$ *and filter function* $\varphi_2(\sigma) = \frac{e^\sigma - \varphi_1(\sigma)}{\sigma}$.

In case of more regular solutions the general scheme (4.12) takes the simplified form

$$\begin{aligned} u^{\ell+1} &= e^{i\tau\Delta}u^\ell \\ &- i\tau e^{i\tau\Delta}\Big((u^\ell)^2\Big(\varphi_1(-2i\tau\Delta)-\frac{1}{2}\Big)\overline{u^\ell}+\frac{1}{2}\Big(e^{i\tau\Delta}u^\ell\Big)^2 e^{i\tau\Delta}\overline{u^\ell}\Big) \\ &- \frac{\tau^2}{2}e^{i\tau\Delta}\Big(|u^\ell|^4u^\ell\Big) \end{aligned} \tag{A.18}$$

with a local error of order $\mathcal{O}(\tau^3\nabla^3 u)$, and for smooth solutions

$$\begin{aligned} u^{\ell+1} = e^{i\tau\Delta}u^\ell - i\tau e^{i\tau\Delta}\Big(\Psi_1 - i\Psi_2\frac{1}{2}\tau\Delta\Big)|u^\ell|^2u^\ell \\ + \frac{\tau^2}{2}e^{i\tau\Delta}\Psi_3\Big(-(u^\ell)^2\Delta\overline{u^\ell}+2|u^\ell|^2\Delta u^\ell-|u^\ell|^4u^\ell\Big) \end{aligned} \tag{A.19}$$

with a local error of order $\mathcal{O}(\tau^3\Delta^2 u)$ and suitable filter functions $\Psi_{1,2,3}$ satisfying

$$\Psi_{1,2,3} = \Psi_{1,2,3}(i\tau\Delta), \quad \Psi_{1,2,3}(0)=1, \quad \|\tau\Psi_{1,2,3}(i\tau\Delta)\Delta\| \le 1.$$

Remark A.4 With the general framework we had recovered at first-order exactly the resonance based first-order scheme (A.3) derived in [67]. The second-order schemes (A.17) and (A.18) are new and allow us to improve the classical local error structure $\mathcal{O}\big(\tau^3\Delta^4 u\big)$. We refer to [58, 29] for the error analysis of classical splitting and exponential integrators for the Schrödinger equation.

The new second-order low regularity scheme (A.17) moreover allows us to improve the recently introduced scheme [57], which only allows for a local error of order $\mathcal{O}\big(\tau^{2+1/2}\Delta u\big)$. Thus we an break the order barrier of $3/2$ previously assumed for resonance based approximations for Schrödinger equations.

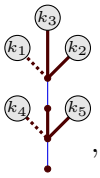
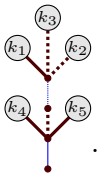
With the new framework we in addition recover for smooth solutions classical second-order Schrödinger approximations obeying the classical local error structure $\mathcal{O}\big(\tau^2\Delta^2 u\big)$: Depending on the choice of filter functions $\Psi_{1,2,3}$ the second-order scheme (A.19) coincides with second-order exponential Runge–Kutta or exponential integrator methods ([7, 18, 46]), see also Remark 4.11 below. The favorable error behavior of the new schemes for non-smooth solutions is underlined by numerical experiments, see Figure 3.

Proof. **Construction of the schemes.** For the second-order scheme we need a local error of order $\mathcal{O}(\tau^3)$. Therefore, we need to choose $r=1$ in Definition 4.4 and the corresponding trees accordingly. This yields that

$$\begin{aligned} U_k^{n,1}(\tau,v) = \frac{\Upsilon^p(X_k)(v)}{S(X_k)}\Pi_n(\mathfrak{D}_1(\mathfrak{I}_{(\mathfrak{t}_1,0)}(X_k)))(\tau) \\ + \sum_{\substack{k_1,k_2,k_3\in\mathbf{Z}^d\\ -k_1+k_2+k_3=k}} \frac{\Upsilon^p(X_kT_1)(v)}{S(T_1)}\Pi_n(\mathfrak{D}_1(\mathfrak{I}_{(\mathfrak{t}_1,0)}(X_kT_1)))(\tau) \end{aligned} \tag{A.20}$$

$$+\sum_{\substack{k_1,k_2,k_3,k_4,k_5\in\mathbf{Z}^d\\ -k_1+k_2+k_3-k_4+k_5=k}}\frac{\Upsilon^p(X_kT_2)(v)}{S(T_2)}\Pi_n(\mathfrak{D}_1(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_2)))(\tau)$$
$$+\sum_{\substack{k_1,k_2,k_3,k_4,k_5\in\mathbf{Z}^d\\ k_1-k_2-k_3+k_4+k_5=k}}\frac{\Upsilon^p(X_kT_3)(v)}{S(T_3)}\Pi_n(\mathfrak{D}_1(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_3)))(\tau)$$

with T_1 defined in (A.9) and

$$\mathcal{T}_0^3(R)=\{T_0,T_1,T_2,T_3,\ k_i\in\mathbf{Z}^d\},\quad T_2=$$  $$,\quad T_3=$$  $$.$$

In symbolic notation one gets

$$\begin{aligned}
T_2&=\mathcal{I}_{(\mathfrak{t}_2,0)}(X_kF_2),\quad k=-k_1+k_2+k_3-k_4+k_5\\
F_2&=\mathcal{I}_{(\mathfrak{t}_1,1)}(X_{k_4})\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{-k_1+k_2+k_3}T_1)\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_5}),\\
T_3&=\mathcal{I}_{(\mathfrak{t}_2,0)}(X_kF_3),\quad k=k_1-k_2-k_3+k_4+k_5\\
F_3&=\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_4})\overline{\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{-k_1+k_2+k_3}T_1)}\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_5}),
\end{aligned}\tag{A.21}$$

where thanks to (4.8)

$$\overline{\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{-k_1+k_2+k_3}T_1)}=\mathcal{I}_{(\mathfrak{t}_1,1)}\big(X_{-k_1+k_2+k_3}\overline{T_1}\big).$$

Note that the trees T_2,T_3 correspond to the next iterated integrals

$$\begin{aligned}
\mathcal{I}_2(v^3,\overline{v}^2,\xi)&=\int_0^\xi e^{-i\xi_1\Delta}\Big[\Big(e^{i\xi_1\Delta}v\Big)\Big(e^{-i\xi_1\Delta}\overline{v}\Big)\Big(e^{i\xi_1\Delta}\mathcal{I}_1(v^2,\overline{v},\xi_1)\Big)\Big]d\xi_1\\
\mathcal{I}_3(v^3,\overline{v}^2,\xi)&=\int_0^\xi e^{-i\xi_1\Delta}\Big[\Big(e^{i\xi_1\Delta}v\Big)^2\Big(e^{-i\xi_1\Delta}\overline{\mathcal{I}_1(v^2,\overline{v},\xi_1)}\Big)\Big]d\xi_1.
\end{aligned}\tag{A.22}$$

The definitions (4.7) imply that

$$\begin{aligned}
\Upsilon^p(X_kT_2)(v)&=2\Upsilon^p(\mathcal{I}_{(\mathfrak{t}_1,1)}(X_{k_4}))(v)\Upsilon^p(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_1))(v)\Upsilon^p(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_5}))(v)\\
&=2\overline{\hat v}_{k_4}\big(2\overline{\hat v}_{k_1}\hat v_{k_2}\hat v_{k_3}\big)\hat v_{k_5}\\
\Upsilon^p(X_kT_3)(v)&=2\Upsilon^p(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_4}))(v)\Upsilon^p\big(X_k\overline{T_1}\big)(v)\Upsilon^p(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_5}))(v)\\
&=2\hat v_{k_4}\overline{\big(2\overline{\hat v}_{k_1}\hat v_{k_2}\hat v_{k_3}\big)}\hat v_{k_5}=2\hat v_{k_4}\big(2\hat v_{k_1}\overline{\hat v}_{k_2}\overline{\hat v}_{k_3}\big)\hat v_{k_5}
\end{aligned}$$

and by (4.6) we obtain

$$S(T_2)=1\cdot2=2,\quad S(T_3)=2\cdot2=4.$$

Next we have to compute $\Pi_n(\mathcal{D}_1(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_j)))$ for $j=1,2,3$.
1. Computation of $\Pi_n(\mathcal{D}_1(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_1)))$: Here $k=-k_1+k_2+k_3$. Similarly to (A.12) we obtain that

$$\Pi_n(\mathcal{D}_1(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_1)))(\tau)=e^{-i\tau k^2}\mathcal{K}^{k,1}_{(\mathfrak{t}_2,1)}\Big(e^{i\xi(k_1^2-k_2^2-k_3^2)},n\Big)(\tau), \tag{A.23}$$

where by (A.13) we have that if $n\geq 4$

$$\mathcal{K}^{k,1}_{(\mathfrak{t}_2,1)}\Big(e^{i\xi(k_1^2-k_2^2-k_3^2)},n\Big)(\tau)=-i\tau+\big(k^2+k_1^2-k_2^2-k_3^2\big)\frac{\tau^2}{2}$$

If $n<4$

$$\mathcal{K}^{k,1}_{(\mathfrak{t}_2,1)}\Big(e^{i\xi(k_1^2-k_2^2-k_3^2)},n\Big)(\tau)=-i\Psi^1_{n,0}(\mathscr{L}_{\text{dom}},0)(\tau)-i\frac{g(\tau)-1}{\tau}\Psi^1_{n,0}(\mathscr{L}_{\text{dom}},1)(\tau),$$

with

$$\Psi^1_{n,0}(\mathscr{L}_{\text{dom}},\ell)(\tau)=\begin{cases}\displaystyle\int_0^\tau \xi^\ell f(\xi)d\xi, & \text{if } 4-\ell>n \text{ and } n<4,\\ \displaystyle\sum_{m\leq 1-\ell}\frac{f^{(m)}(0)}{m!}\int_0^\tau \xi^{\ell+m}d\xi, & \text{if } 4-\ell\leq n \text{ and } n<4.\end{cases}$$

Hence,

$$\begin{aligned}
\Pi_{n=2}(\mathcal{D}_1(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_1)))(\tau)&=-i\tau e^{-i\tau k^2}\Big(\varphi_1(2i\tau k_1^2)+(g(\tau)-1)\varphi_2(2i\tau k_1^2)\Big)\\
\Pi_{n=3}(\mathcal{D}_1(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_1)))(\tau)&=-i\tau e^{-i\tau k^2}\Big(\varphi_1(2i\tau k_1^2)+\frac{1}{2}(g(\tau)-1)\Big)\\
\Pi_{n\geq 4}(\mathcal{D}_1(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_1)))(\tau)&=e^{-i\tau k^2}\Big(-i\tau+\big(k^2+k_1^2-k_2^2-k_3^2\big)\frac{\tau^2}{2}\Big)
\end{aligned} \tag{A.24}$$

where $g(\tau)=e^{i\tau(k^2-k_1^2-k_2^2-k_3^2)}$ and $\mathscr{L}(k)=\mathscr{L}_{\text{dom}}(k)+\mathscr{L}_{\text{low}}(k)$.
2. Computation of $\Pi_n(\mathcal{D}_1(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_2)))$: Here $k=-k_1+k_2+k_3-k_4+k_5$. By (3.2) and $P_{\mathfrak{t}_1}(k)=-k^2$ we have

$$\begin{aligned}
\Pi_n(\mathcal{D}_1(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_2)))(\tau)&=e^{-i\tau k^2}(\Pi_n\mathcal{D}_1(T_2))(\tau)=e^{-i\tau k^2}\big(\Pi_n\mathcal{I}^1_{(\mathfrak{t}_2,0)}(X_kF_2)\big)(\tau)\\
&=e^{-i\tau k^2}\mathcal{K}^{k,1}_{(\mathfrak{t}_2,0)}(\Pi_n(\mathcal{D}_0(F_2)),n)(\tau).
\end{aligned}$$

Furthermore, by the mulitiplicativity of Π_n we obtain with the aid of (A.12) and (A.1.1)

$$\begin{aligned}
\Pi_n(\mathcal{D}_0(F_2))(\tau)&=\big(\Pi_n\mathcal{I}^0_{(\mathfrak{t}_1,1)}(X_{k_4})\big)(\tau)\big(\Pi_n\mathcal{I}^0_{(\mathfrak{t}_1,0)}(X_kT_1)\big)(\tau)\big(\Pi_n\mathcal{I}^0_{(\mathfrak{t}_1,0)}(X_{k_5})\big)(\tau)\\
&=e^{-i\tau k_4^2}e^{-i\tau(-k_1+k_2+k_3)^2}\mathcal{K}^{-k_1+k_2+k_3,0}_{(\mathfrak{t}_2,0)}\Big(e^{i\xi(k_1^2-k_2^2-k_3^2)},n\Big)(\tau)e^{-i\tau k_5^2}\\
&=-ie^{-i\tau(k_4^2+k_5^2)}e^{-i\tau(-k_1+k_2+k_3)^2}\Psi^0_{n,0}(\mathscr{L}_{\text{dom}},0)(\tau),
\end{aligned}$$

where by (A.14) and the fact that $n \geq 2$ we have that

$$\Psi^0_{n,0}(\mathscr{L}_{\text{dom}}, 0)(\tau) = \tau.$$

Hence,

$$\begin{aligned}\Pi_n\big(\mathscr{I}^1_{(\mathfrak{t}_1,0)}(X_k T_2)\big)(\tau) &= -ie^{-i\tau k^2}\mathscr{K}^{k,1}_{(\mathfrak{t}_2,0)}\Big(\xi e^{-i\xi(k_4^2+k_5^2)}e^{-i\xi(-k_1+k_2+k_3)^2}, n\Big)(\tau)\\ &= -e^{-i\tau k^2}\frac{\tau^2}{2}\end{aligned}$$

where we used again that $n \geq 2$.

3. Computation of $\Pi_n(\mathscr{D}_1(\mathscr{I}_{(\mathfrak{t}_1,0)}(X_k T_3)))$: Here $k = k_1 - k_2 - k_3 + k_4 + k_5$. Similarly we can show that

$$\Pi_n(\mathscr{D}_1(\mathscr{I}_{(\mathfrak{t}_1,0)}(X_k T_3)))(\tau) = +e^{-i\tau k^2}\frac{\tau^2}{2}.$$

Plugging the results from Computations 1–3 into (A.20) yields that

$$\begin{aligned}U^{n,1}_k(\tau, v) &= e^{-i\tau k^2}\hat{v}_k \\ &\quad - i\tau \sum_{-k_1+k_2+k_3=k} e^{-i\tau k^2}\frac{1}{\tau}\Pi_n\big(\mathscr{I}^1_{(\mathfrak{t}_1,0)}(X_k T_1)\big)(\tau)\,\overline{\hat{v}}_{k_1}\hat{v}_{k_2}\hat{v}_{k_2} \\ &\quad - \frac{\tau^2}{2}\sum_{-k_1+k_2+k_3-k_4+k_5=k} e^{-i\tau k^2}\overline{\hat{v}}_{k_1}\hat{v}_{k_2}\hat{v}_{k_2}\overline{\hat{v}}_{k_4}\hat{v}_{k_5}\end{aligned} \tag{A.25}$$

with $\Pi_n(\mathscr{D}_1(\mathscr{I}_{(\mathfrak{t}_1,0)}(X_k T_1)))$ given in (A.24) and we have used that the last two sums in (A.20) can be merged into one. The Fourier based resonance schemes (A.25) can easily be transformed back to physical space yielding the three low-to-high regularity second-order iterative schemes (A.17) – (A.19) which depend on the smoothness n of the exact solution.

Local error analysis. It remains to show that the general local error bound given in Theorem 4.7 implies the sharp local error estimates

$$\mathcal{O}\big(\tau^3\nabla^n\big), \quad n = 2, 3, 4 \tag{A.26}$$

of the schemes (A.17) – (A.19). Theorem 4.7 implies that

$$U^{n,1}_k(\tau, v) - U^1_k(\tau, v) = \sum_{T\in\mathcal{T}^3_0(R)} \mathcal{O}\big(\tau^3\mathscr{L}^1_{\text{low}}(T, n)\Upsilon^p(X_k T)(v)\big) \tag{A.27}$$

with $T_0 = \mathbf{1}$, T_1 given in (A.9) and T_2, T_3 defined in (A.21).

1) Computation of $\mathscr{L}^1_{\text{low}}(T_0, n)$ and $\mathscr{L}^1_{\text{low}}(T_1, n)$:
By Definition 3.9 we obtain similarly to the first-order scheme (here with $r = 1$) that

$$\mathscr{L}^1_{\text{low}}(T_0, n) = 1, \quad \mathscr{L}^1_{\text{low}}(T_1, n) = k^{\max(n,2)} = k^{\max(n,2)}.$$

2) Computation of $\mathscr{L}^1_{\text{low}}(T_2, n)$:
Next we calculate that

$$\mathscr{L}^1_{\text{low}}(T_2, n) = \mathscr{L}^1_{\text{low}}(\mathscr{I}_{(\mathfrak{t}_2,0)}(X_k F_2), n) = \mathscr{L}^0_{\text{low}}(F_2, n) + \sum_j k^{\bar{n}_j} \tag{A.28}$$

with

$$\bar{n}_j = \max(n, \deg(\mathscr{R}_{\text{low}}(\mathscr{I}_{(\mathfrak{t}_2,0)}(X_k F_2^j))^2))$$

where $\sum_j F_2^j = \mathscr{M}_{(1)}\Delta\mathscr{D}_{r-1}(F_2)$ where we have $r = 1$ here. Hence, we have to calculate $\Delta\mathscr{D}_0(F_2)$. By the multiplicativity of the coproduct, its recursive defintion (2.19) and the calculation of $\mathscr{D}_r(T_1)$ given in (2.20) we obtain that

$$\begin{aligned}
\Delta\mathscr{D}_r(F_2) &= \Delta\mathscr{I}^r_{(\mathfrak{t}_1,1)}(X_{k_4})\Delta\mathscr{I}^r_{(\mathfrak{t}_1,0)}(X_{-k_1+k_2+k_3}T_1)\Delta\mathscr{I}^r_{(\mathfrak{t}_1,0)}(X_{k_5}) \\
&= \big(\mathscr{I}^r_{(\mathfrak{t}_1,1)}(X_{k_4}) \otimes \mathbf{1}\big)\big(\mathscr{I}^r_{(\mathfrak{t}_1,0)}(X_{-k_1+k_2+k_3}\cdot) \otimes \mathrm{id}\big) \\
&\qquad \Delta\mathscr{D}_r(T_1))\big(\mathscr{I}^r_{(\mathfrak{t}_1,0)}(X_{k_5}) \otimes \mathbf{1}\big) \\
&= \mathscr{D}_r(F_2) \otimes \mathbf{1} \\
&\quad + \mathscr{I}^r_{(\mathfrak{t}_1,1)}(X_{k_4})\mathscr{I}^r_{(\mathfrak{t}_1,0)}(X_{k_5})\mathscr{I}^r_{(\mathfrak{t}_1,0)}\left(\sum_{m\le r+1} \frac{X^m_{-k_1+k_2+k_3}}{m!}\right) \otimes \mathscr{D}_{(r,m)}(T_1)
\end{aligned}$$

Hence, as $r = 1$

$$\sum_{j=1}^4 F_2^j = \mathscr{D}_0(F_2) + \sum_{m\le r+1} \frac{1}{m!}\mathscr{I}^0_{(\mathfrak{t}_1,1)}(X_{k_4})\mathscr{I}^0_{(\mathfrak{t}_1,0)}(X_{k_5})\mathscr{I}^0_{(\mathfrak{t}_1,0)}\big(X^m_{-k_1+k_2+k_3}\big)$$

Now we are in the position to compute $\bar{n}_1$: By Definition 2.5 we have

$$\begin{aligned}
\mathscr{R}_{\text{dom}}(\mathscr{I}_{(\mathfrak{t}_2,0)}(X_k F_2)) &= \mathscr{P}_{\text{dom}}(P_{(\mathfrak{t}_2,0)}(k) + \mathscr{R}_{\text{dom}}(F_2)) \\
&= \mathscr{P}_{\text{dom}}\big(k^2 + \mathscr{R}_{\text{dom}}(F_2)\big).
\end{aligned} \tag{A.29}$$

where we used that $P_{\mathfrak{t}_2}(k) = +k^2$ as well as (2.4). Furthermore, we have that

$$\begin{aligned}
\mathscr{R}_{\text{dom}}(F_2) = \mathscr{R}_{\text{dom}}(\mathscr{I}_{(\mathfrak{t}_1,1)}(X_{k_4})) + \mathscr{R}_{\text{dom}}(\mathscr{I}_{(\mathfrak{t}_1,0)}(X_{-k_1+k_2+k_3}T_1)) \\
+ \mathscr{R}_{\text{dom}}(\mathscr{I}_{(\mathfrak{t}_1,0)}(X_{k_5}))
\end{aligned}$$

with

$$\mathscr{R}_{\text{dom}}(\mathscr{I}_{(\mathfrak{t}_1,1)}(X_{k_4})) = P_{(\mathfrak{t}_1,1)}(k_4) + \mathscr{R}_{\text{dom}}(\mathbf{1}) = -P_{\mathfrak{t}_1}(-k_4) = +k_4^2$$

where we used that $P_{\mathfrak{t}_1}(k) = -k^2$ as well as (2.4). Similarly we obtain that

$$\mathscr{R}_{\text{dom}}(\mathscr{I}_{(\mathfrak{t}_1,0)}(X_{k_5})) = -k_5^2.$$

Furthermore, we have that

$$\mathscr{R}_{\text{dom}}(\mathscr{I}_{(\mathfrak{t}_1,0)}(X_{-k_1+k_2+k_3}T_1)) = -(-k_1+k_2+k_3)^2 + \mathscr{R}_{\text{dom}}(T_1)$$

$$= -(-k_1 + k_2 + k_3)^2 + 2k_1^2$$

where we used Example 4. Hence,

$$\mathscr{R}_{\text{dom}}(F_2) = -(-k_1 + k_2 + k_3)^2 + 2k_1^2 + k_4^2 - k_5^2.$$

Plugging this into (A.29) yields

$$\mathscr{R}_{\text{dom}}(\mathscr{I}_{(\mathfrak{t}_2,0)}(X_k F_2)) = \mathscr{P}_{\text{dom}}\big(k^2 - (-k_1 + k_2 + k_3)^2 + 2k_1^2 + k_4^2 - k_5^2\big).$$

Therefore, $\mathscr{R}_{\text{low}}(\mathscr{I}_{(\mathfrak{t}_2,0)}(X_k F_2)) = k$ such that

$$\overline{n}_1 = \max(n, \deg(k^2)) = \max(n, 2).$$

Next we compute $\overline{n}_2$:

$$\mathscr{R}_{\text{dom}}\big(\mathscr{I}_{(\mathfrak{t}_2,0)}\big(X_k F_2^2\big)\big) = \mathscr{P}_{\text{dom}}\big(k^2 + \mathscr{R}_{\text{dom}}\big(F_2^2\big)\big)$$

with

$$\begin{aligned}\mathscr{R}_{\text{dom}}\big(F_2^2\big) = \mathscr{R}_{\text{dom}}(\mathscr{I}_{(\mathfrak{t}_1,1)}(X_{k_4})) + \mathscr{R}_{\text{dom}}(\mathscr{I}_{(\mathfrak{t}_1,0)}(X_{k_5}))\\ + \mathscr{R}_{\text{dom}}(\mathscr{I}_{(\mathfrak{t}_1,0)}(X_{-k_1+k_2+k_3}))\end{aligned}$$

Note that

$$\begin{aligned}\mathscr{R}_{\text{dom}}\big(\mathscr{I}_{(\mathfrak{t}_1,0)}\big(X^m_{-k_1+k_2+k_3}\big)\big) &= \mathscr{R}_{\text{dom}}(\mathscr{I}_{(\mathfrak{t}_1,0)}(X_{-k_1+k_2+k_3}))\\ &= -(-k_1 + k_2 + k_3)^2.\end{aligned}$$

Together with the previous computations we can thus conclude that

$$\mathscr{R}_{\text{dom}}\big(\mathscr{I}_{(\mathfrak{t}_2,0)}\big(X_k F_2^2\big)\big) = \mathscr{P}_{\text{dom}}\big(k^2 - (-k_1 + k_2 + k_3)^2 + k_4^2 - k_5^2\big).$$

Therefore, $\mathscr{R}_{\text{low}}\big(\mathscr{I}_{(\mathfrak{t}_2,0)}\big(X_k F_2^2\big)\big) = k$ and

$$\bar{n}_2 = \max(n, 2).$$

Hence

$$\bar{n}_1 = \bar{n}_2 = \bar{n}_3 = \bar{n}_4 = \max(n, 2).$$

Furthermore, by Definition 3.9 we have

$$\begin{aligned}\mathscr{L}^1_{\text{low}}(F_2, n) &= \mathscr{L}^1_{\text{low}}(\mathscr{I}_{(\mathfrak{t}_1,1)}(X_{k_4}), n) + \mathscr{L}^1_{\text{low}}(\mathscr{I}_{(\mathfrak{t}_1,0)}(X_{-k_1+k_2+k_3} T_1), n)\\ &\quad + \mathscr{L}^1_{\text{low}}(\mathscr{I}_{(\mathfrak{t}_1,0)}(X_{k_5}), n)\\ &= \mathscr{L}^1_{\text{low}}(\mathbf{1}) + \mathscr{L}^1_{\text{low}}(T_1, n) + \mathscr{L}^1_{\text{low}}(\mathbf{1})\\ &= 2 + k^{\max(n,2)}.\end{aligned}$$

Plugging this into (A.28) yields that

$$\mathscr{L}^1_{\text{low}}(T_2, n) = \mathcal{O}\big(k^{\max(n,2)}\big).$$

3) Computation of $\mathscr{L}^1_{\text{low}}(T_3, n)$:
Similarly we obtain that

$$\mathscr{L}^1_{\text{low}}(T_3, n) = \mathcal{O}\big(k^{\max(n,2)}\big).$$

Plugging the computations 1-3 into (A.27) we recover the local error structure (A.26).

□

A.2 Korteweg–de Vries

We consider the Korteweg–de Vries (KdV) equation

$$\partial_t u + \partial_x^3 u = \frac{1}{2}\partial_x u^2 \tag{A.30}$$

with mild solution given by Duhamel's formula

$$u(\tau) = e^{-\tau\partial_x^3} v + \frac{1}{2} e^{-\tau\partial_x^3} \int_0^\tau e^{\xi\partial_x^3} \partial_x u^2(\xi) d\xi.$$

The KdV equation (A.30) fits into the general framework (1.1) with

$$\mathscr{L}\left(\nabla, \frac{1}{\varepsilon}\right) = i\partial_x^3, \quad \alpha = 1 \quad \text{and} \quad p(u, \overline{u}) = p(u) = i\frac{1}{2}u^2.$$

Here $\mathscr{L} = \{\mathfrak{t}_1, \mathfrak{t}_2\}$, $P_{\mathfrak{t}_1} = -X^3$ and $P_{\mathfrak{t}_2} = X^3$. Then, we denoted by | an edge decorated by $(\mathfrak{t}_1, 0)$ and by | an edge decorated by $(\mathfrak{t}_2, 0)$. Following the formalism given in [12], one can provide the rules that generate the trees obtained by iterating the Duhamel formulation:

$$R(|) = \{(|, |)\}\ , \quad R(|) = \{(|), ()\}\ .$$

The general framework (4.12) derived in Section 4 builds the foundation of the first- and second-order resonances based schemes presented below for the KdV equation (A.30). The structure of the schemes depends on the regularity of the solution.

Corollary A.5 *For the KdV equation (A.30) the general scheme (4.12) takes at first order the form*

$$u^{\ell+1} = e^{-\tau\partial_x^3} u^\ell + \frac{1}{6}\left(e^{-\tau\partial_x^3}\partial_x^{-1} u^\ell\right)^2 - \frac{1}{6} e^{-\tau\partial_x^3}\left(\partial_x^{-1} u^\ell\right)^2 \tag{A.31}$$

with a local error of order $\mathcal{O}\left(\tau^2\partial_x^2 u\right)$ *and at second-order*

$$\begin{aligned} u^{\ell+1} &= e^{-\tau\partial_x^3}u^\ell + \frac{1}{6}\left(e^{-\tau\partial_x^3}\partial_x^{-1}u^\ell\right)^2 - \frac{1}{6}e^{-\tau\partial_x^3}\left(\partial_x^{-1}u^\ell\right)^2 \\ &\quad + \frac{\tau^2}{4}e^{-\tau\partial_x^3}\Psi(i\tau\partial_x^2)\left(\partial_x\left(u^\ell\partial_x(u^\ell u^\ell)\right)\right) \end{aligned} \tag{A.32}$$

with a local error of order $\mathcal{O}\left(\tau^3\partial_x^4 u\right)$ *and a suitable filter function* Ψ *satisfying*

$$\Psi = \Psi\left(i\tau\partial_x^2\right), \quad \Psi(0) = 1, \quad \|\tau\Psi\left(i\tau\partial_x^2\right)\partial_x^2\|_r \leq 1.$$

Remark A.6 Note that the first-order scheme (A.31) which was originally derived in [47] is optimised as the resonance structure factorises in such a way that all frequencies can be integrated exactly (details are given in the proof). This is in general true, for equations in one dimension with quadratic nonlinearities up to first order. However, this trick can not be applied to derive second-order methods. The second-order scheme is new and allows us to improve the local error structure $\mathcal{O}\left(\tau^3\partial_x^5 u\right)$ introduced by the classical Strang splitting scheme [49]. Due to the stability constrain induced by Burger's nonlinearity it is preferable to embed the resonance structure into the numerical discretisation even for smooth solutions. In Figure 4 we numerically observe the favourable error behaviour of the new resonance based scheme (A.32) for $\mathscr{C}^\infty$ solutions.

Proof. The proof follows the line of argumentation to the analysis for the Schrödinger equation. The construction of the schemes is again based on the general framework (4.12). Hence, we have to consider for $r = 0, 1$

$$U_k^{n,r}(\tau, v) = \sum_{T\in\mathcal{T}_0^{r+2}(R)} \frac{\Upsilon^p(X_kT)(v)}{S(T)}\Pi_n(\mathfrak{D}_r(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT)))(\tau). \tag{A.33}$$

Thereby, for the first-order scheme the trees of interests are

$$\mathcal{T}_0^2(R) = \{T_0, T_1,\ k_i \in \mathbf{Z}^d\}, \quad T_0 = \mathbf{1} \quad \text{and} \quad T_1 = \quad$$

where T_1 is associated to the first-order iterated integral

$$\mathcal{I}_1(v^2, s) = \int_0^s e^{s_1\partial_x^3}\partial_x(e^{-s_1\partial_x^3}v)^2 ds_1$$

and in symbolic notation takes the form

$$T_1 = \mathcal{I}_{(\mathfrak{t}_2,0)}(X_kF_1) \quad F_1 = \mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_1})\mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_2}) \quad \text{with } k = k_1 + k_2.$$

For the first-order scheme we set $r = 0$ in (A.42) such that

$$U_k^{n,0}(\tau, v) = \frac{\Upsilon^p(X_kT_0)(v)}{S(T_0)}\Pi_n(\mathfrak{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_kT_0)))(\tau) \tag{A.34}$$

$$+ \sum_{k=k_1+k_2} \frac{\Upsilon^p(X_k T_1)(v)}{S(T_1)} \Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k T_1)))(\tau).$$

For the first term we readily obtain that

$$\frac{\Upsilon^p(X_k T_0)(v)}{S(T_0)} \Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k T_0)))(\tau) = e^{-i\tau k^3} \hat{v}_k.$$

It remains to compute the second term. Note that thanks to (3.2) we have that

$$\begin{aligned} \Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k T_1)))(\tau) &= e^{i\tau P_{\mathfrak{t}_1}(k)} \Pi_n(\mathcal{D}_0(T_1))(\tau) \\ &= e^{-i\tau k^3} \Pi_n(\mathcal{I}^0_{(\mathfrak{t}_2,0)}(X_k F_1))(\tau) \\ &= e^{-i\tau k^3} \mathcal{K}^{k,0}_{(\mathfrak{t}_2,0)}(\Pi_n(\mathcal{D}_{-1}(F_1)))(\tau). \end{aligned} \tag{A.35}$$

By the product formula we furthermore obtain that

$$\begin{aligned} \Pi_n(\mathcal{D}_{-1}(F_1))(\tau) &= \Pi_n\Big(\mathcal{I}^{-1}_{(\mathfrak{t}_1,0)}(X_{k_1})\Big)(\tau) \Pi_n\Big(\mathcal{I}^{-1}_{(\mathfrak{t}_1,0)}(X_{k_2})\Big)(\tau) \\ &= e^{-i\tau k_1^3} e^{-i\tau k_2^3}. \end{aligned}$$

Plugging the above relation into (A.35) yields that

$$\Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k T_1)))(\tau) = e^{-i\tau k^3} \mathcal{K}^{k,0}_{(\mathfrak{t}_2,0)}\Big(e^{i\xi(-k_1^3-k_2^3)}\Big)(\tau).$$

Next we observe that

$$P_{(\mathfrak{t}_2,0)}(k) - k_1^3 - k_2^3 = k^3 - k_1^3 - k_2^3 = 3k_1k_2(k_1+k_2)$$

such that

$$\frac{1}{P_{(\mathfrak{t}_2,0)}(k) - k_1^3 - k_2^3}$$

can be mapped back to physical space. Therefore, we set

$$\mathscr{L}_{\text{dom}} = P_{(\mathfrak{t}_2,0)}(k) - k_1^3 - k_2^3 = 3k_1k_2(k_1+k_2)$$

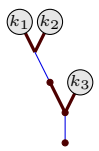
and integrate all frequencies exactly. This implies

$$\begin{aligned} \Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k T_1)))(\tau) &= e^{-i\tau k^3} \frac{i(k_1+k_2)}{3ik_1k_2(k_1+k_2)} \Big(e^{i\tau(k^3-k_1^3-k_2^3)} - 1\Big) \\ &= \frac{1}{3k_1k_2}\Big(e^{-i\tau(k_1^3+k_2^3)} - e^{-i\tau k^3}\Big). \end{aligned}$$

Together with (A.42) this yields the scheme (A.31).

For the second-order scheme we need to take into account the following trees

$$\mathcal{T}_0^3(R) = \{T_0, T_1, T_2,\ k_i \in \mathbf{Z}^d\}, \quad T_2 = \quad$$



which is associated to the second-order iterated integral

$$\mathcal{J}_2(v^3,s)=\int_0^s e^{s_1\partial_x^3}\partial_x\bigg((e^{-s_1\partial_x^3}v)e^{-s_1\partial_x^3}\int_0^{s_1}e^{s_2\partial_x^3}\partial_x(e^{-s_2\partial_x^3}v)^2ds_2\bigg)ds_1.$$

Then one can proceed as in the second-order schemes for the Schrödinger equation. We omit the details here. The local error analysis is then given by Theorem 4.7 noting that $\alpha=1$ and

$$\mathscr{L}^0_{\text{low}}(T_1,\cdot)=k^{1+\alpha},\quad \mathscr{L}^1_{\text{low}}(T_1,\cdot)=\mathscr{L}^1_{\text{low}}(T_2,\cdot)=k^{2(1+\alpha)}.$$

□

A.3 Klein–Gordon

In this section we apply the general framework (4.12) to the Klein–Gordon equation

$$\partial_t^2 z-\Delta z+\frac{1}{\varepsilon^2}z=|z|^2z,\quad z(0,x)=\gamma(x),\quad \partial_t z(0,x)=\frac{1}{\varepsilon^2}\delta(x). \tag{A.36}$$

Here we are in particular interested in resolving the highly oscillatory, so-called non-relativistic, structure of the PDE when the speed of light $c=\frac{1}{\varepsilon}$ formally tends to infinity.

Via the tranformation $u=z-i\varepsilon\langle\nabla\rangle_{\frac{1}{\varepsilon}}^{-1}\partial_t z$ we express (A.36) in its first-order form

$$i\partial_t u=-\frac{1}{\varepsilon}\langle\nabla\rangle_{\frac{1}{\varepsilon}}u+\frac{1}{\varepsilon}\langle\nabla\rangle_{\frac{1}{\varepsilon}}^{-1}\tfrac{1}{8}(u+\overline{u})^3,\qquad \tfrac{1}{\varepsilon}\langle\nabla\rangle_{\frac{1}{\varepsilon}}=\tfrac{1}{\varepsilon}\sqrt{\tfrac{1}{\varepsilon^2}-\Delta}. \tag{A.37}$$

The first-order form (A.37) casts into the general form (1.1) with

$$\mathscr{L}\bigg(\nabla,\frac{1}{\varepsilon}\bigg)=\frac{1}{\varepsilon}\langle\nabla\rangle_{\frac{1}{\varepsilon}},\quad \alpha=0\quad\text{and}\quad p(u,\overline{u})=\frac{1}{\varepsilon}\langle\nabla\rangle_{\frac{1}{\varepsilon}}^{-1}\tfrac{1}{8}(u+\overline{u})^3.$$

The leading operator $\mathscr{L}\big(\nabla,\frac{1}{\varepsilon}\big)$ thereby triggers oscillations of type

$$\sum_{\ell\in\mathbf{Z}}e^{it\ell\frac{1}{\varepsilon^2}}$$

which can be formally seen by the Taylor series expansion

$$\mathscr{L}\bigg(\nabla,\frac{1}{\varepsilon}\bigg)=\frac{1}{\varepsilon}\langle\nabla\rangle_{\frac{1}{\varepsilon}}=\frac{1}{\varepsilon^2}-\frac{1}{2}\Delta+\mathcal{O}\bigg(\frac{\Delta^2}{\varepsilon^2}\bigg).$$

In oder to determine these dominant oscillations we define the non-oscillatory operators

$$\mathscr{B}_\Delta=\frac{1}{\varepsilon}\langle\nabla\rangle_{\frac{1}{\varepsilon}}-\frac{1}{\varepsilon^2},\qquad \mathscr{B}_\Delta(k)=\frac{1}{\varepsilon^2}\sqrt{1+\frac{k^2}{\varepsilon^2}}-\frac{1}{\varepsilon^2} \tag{A.38}$$

$$\mathscr{C}_\Delta = \frac{1}{\varepsilon}\langle\nabla\rangle^{-1}_{\frac{1}{\varepsilon}}, \qquad \mathscr{C}_\Delta(k) = \frac{1}{\sqrt{1+\frac{k^2}{\varepsilon^2}}}$$

which both can be uniformly bounded in ε thanks to the estimates $\|\mathscr{B}_\Delta w\| \leq \frac{1}{2}\|\Delta w\|$, $\frac{1}{1+x^2} \leq 1$. The latter motivates us to rewrite the oscillatory equation (A.37) in the following form

$$i\partial_t u = -\left(\frac{1}{\varepsilon^2} + \mathscr{B}_\Delta\right)u + \mathscr{C}_\Delta \tfrac{1}{8}(u+\overline{u})^3. \tag{A.39}$$

Here $\mathscr{L} = \{\mathfrak{t}_1, \mathfrak{t}_2\}$, $P_{\mathfrak{t}_1} = -\left(\frac{1}{\varepsilon^2} + \mathscr{B}_\Delta(X)\right)$ and $P_{\mathfrak{t}_2} = \frac{1}{\varepsilon^2} + \mathscr{B}_\Delta(X)$. Then, we denoted by | an edge decorated by $(\mathfrak{t}_1, 0)$, ⋮ an edge denoted by $(\mathfrak{t}_1, 1)$ by | an edge decorated by $(\mathfrak{t}_2, 0)$ and by | an edge decorated by $(\mathfrak{t}_2, 1)$. The rules that generate the trees obtained by iterating the Duhamel formulation are given by:

$$\begin{aligned}
R(|) &= \{(|,|,|),(|,|,⋮),(|,⋮,⋮),(⋮,⋮,⋮),\}\ ,\\
R(|) &= \{(|,|,|),(|,|,⋮),(|,⋮,⋮),(⋮,⋮,⋮),\}\ ,\\
R(|) &= \{(|),()\}\ , \quad R(⋮) = \{(|),()\}\ .
\end{aligned}$$

A.3.1 First-order scheme

The general framework (4.12) derived in Section 4 builds the foundation of the first-order resonance based schemes presented below for the Klein–Gordon equation equation (A.37).

Corollary A.7 *For the Klein–Gordon equation (A.37) the general scheme (4.12) takes at first order the form*

$$\begin{aligned}
u^{\ell+1} = {} & e^{i\tau\left(\frac{1}{\varepsilon^2}+\mathscr{B}_\Delta\right)}u^\ell - \tau\frac{3i}{8}e^{i\tau\left(\frac{1}{\varepsilon^2}+\mathscr{B}_\Delta\right)}\mathscr{C}_\Delta|u^\ell|^2u^\ell \\
& - \tau\frac{i}{8}e^{i\tau\left(\frac{1}{\varepsilon^2}+\mathscr{B}_\Delta\right)}\mathscr{C}_\Delta\left(\varphi_1\left(2i\frac{1}{\varepsilon^2}\tau\right)\left(u^\ell\right)^3 + 3\varphi_1\left(-2i\frac{1}{\varepsilon^2}\tau\right)\left|u^\ell\right|^2u^\ell\right. \\
& \left. + \varphi_1\left(-4i\frac{1}{\varepsilon^2}\tau\right)\left(\overline{u^\ell}\right)^3\right)
\end{aligned} \tag{A.40}$$

with a local error $\mathcal{O}\left(\tau^2\Delta u\right)$ *and the filter function* $\varphi_1(\sigma) = \frac{e^\sigma-1}{\sigma}$.

If we allow step size restrictions $\tau = \tau\left(\frac{1}{\varepsilon^2}\right)$ *the general scheme (4.12) takes the simplified form*

$$u^{\ell+1} = e^{i\tau\left(\frac{1}{\varepsilon^2}+\mathscr{B}_\Delta\right)}u^\ell - \tau\frac{i}{8}e^{i\tau\left(\frac{1}{\varepsilon^2}+\mathscr{B}_\Delta\right)}\mathscr{C}_\Delta\left(u^\ell+\overline{u^\ell}\right)^3 \tag{A.41}$$

with a local error of order $\mathcal{O}\left(\frac{\tau^2}{\varepsilon^2}u\right) + \mathcal{O}(\tau^2\Delta u)$.

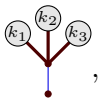
Remark A.8 With the general framework we recover at first-order exactly the resonance based first-order scheme (A.40) derived in [5]. If we allow for step size restrictions, we recover a classical approximation the classical local error structure $\mathcal{O}\left(\frac{\tau^2}{\varepsilon^2}\right)$ introduced by classical Strang splitting or Gautschi-type schemes ([3]).

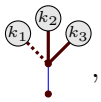
Proof. From the general framework (4.12) (with $r = 0$) we obtain that

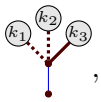
$$U_k^{n,0}(\tau, v) = \sum_{T \in \mathcal{T}_0^2(R)} \frac{\Upsilon^p(X_k T)(v)}{S(T)} \Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k T)))(\tau). \tag{A.42}$$

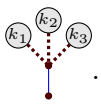
with

$$\mathcal{T}_0^2(R) = \{T_0, T_1, T_2, T_3, T_4,\, k_i \in \mathbf{Z}^d\}, \quad T_0 = \mathbf{1}$$

$T_1 =$ 

, $T_2 =$ 

, $T_3 =$ 

, $T_4 =$ 

.

Let us carry out the computation for the tree T_1 which in symbolic notation takes the form

$$\begin{aligned} T_1 &= \mathcal{I}_{(\mathfrak{t}_2,0)}(X_k F_1), \quad k = k_1 + k_2 + k_3. \\ F_1 &= \mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_1}) \mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_2}) \mathcal{I}_{(\mathfrak{t}_1,0)}(X_{k_3}) \end{aligned}$$

Thanks to (3.2) and the fact that $P_{(\mathfrak{t}_1,0)}\left(k, \frac{1}{\varepsilon^2}\right) = \frac{1}{\varepsilon^2} + \mathcal{B}_\Delta(k)$ we obtain

$$\begin{aligned} \Pi_n(\mathcal{D}_r(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k T_1)))(\tau) &= e^{i\tau P_{(\mathfrak{t}_1,0)}(k, \frac{1}{\varepsilon})}(\Pi_n \mathcal{D}_0(T_1))(\tau) \\ &= e^{i\tau\left(\frac{1}{\varepsilon^2} + \mathcal{B}_\Delta(k)\right)}(\Pi_n \mathcal{I}^0_{(\mathfrak{t}_2,0)}(X_k F_1))(\tau) \\ &= e^{i\tau\left(\frac{1}{\varepsilon^2} + \mathcal{B}_\Delta(k)\right)} \mathcal{K}^{k,0}_{(\mathfrak{t}_2,0)}(\Pi_n \mathcal{D}_{-1}(F_1))(\tau). \end{aligned}$$

By the product rule we furthermore have that

$$\begin{aligned} \Pi_n \mathcal{D}_{-1}(F_1)(\xi) &= \left(\Pi_n \mathcal{I}^{-1}_{(t_1,0)} X_{k_1}\right)(\xi)\left(\Pi_n \mathcal{I}^{-1}_{(t_1,0)} X_{k_2}\right)(\xi)\left(\Pi_n \mathcal{I}^{-1}_{(t_1,0)} X_{k_3}\right)(\xi) \\ &= e^{i\xi\left(3\frac{1}{\varepsilon^2} + \mathcal{B}_\Delta(k_1) + \mathcal{B}_\Delta(k_2) + \mathcal{B}_\Delta(k_3)\right)} \end{aligned}$$

such that

$$\begin{aligned} &\Pi_n(\mathcal{D}_0(\mathcal{I}_{(\mathfrak{t}_1,0)}(X_k T_1)))(\tau) \\ &\quad = e^{i\tau\left(\frac{1}{\varepsilon^2} + \mathcal{B}_\Delta(k)\right)} \mathcal{K}^{k,0}_{(\mathfrak{t}_2,0)}\left(e^{i\xi\left(3\frac{1}{\varepsilon^2} + \mathcal{B}_\Delta(k_1) + \mathcal{B}_\Delta(k_2) + \mathcal{B}_\Delta(k_3)\right)}\right)(\tau). \end{aligned} \tag{A.43}$$

Definition 3.1 together with Remark 2.6 and the observation $P_{(\mathfrak{t}_2,0)}\left(k, \frac{1}{\varepsilon^2}\right) = -\left(\frac{1}{\varepsilon^2} + \mathcal{B}_\Delta(k)\right)$ implies that

$$\mathcal{L}_{\text{dom}} = \mathcal{P}_{\text{dom}}\left(P_{(\mathfrak{t}_2,0)}\left(k, \frac{1}{\varepsilon^2}\right) + P\right) \tag{A.44}$$

$$= \mathscr{P}_{\text{dom}}\left(2\frac{1}{\varepsilon^2} - \mathscr{B}_\Delta(k) + \mathscr{B}_\Delta(k_1) + \mathscr{B}_\Delta(k_2) + \mathscr{B}_\Delta(k_3)\right) = 2\frac{1}{\varepsilon^2}.$$

Hence,

$$\mathscr{K}^{k,0}_{(\mathfrak{t}_2,0)}\left(e^{i\xi\left(3\frac{1}{\varepsilon^2}+\mathscr{B}_\Delta(k_1)+\mathscr{B}_\Delta(k_2)+\mathscr{B}_\Delta(k_3)\right)}\right)(\tau) = -i\frac{1}{8}\mathscr{C}_\Delta(k)\frac{e^{2i\tau\frac{1}{\varepsilon^2}}-1}{2i\frac{1}{\varepsilon^2}}.$$

Plugging this into (A.43) yields that

$$\Pi_n(\mathscr{D}_0(\mathscr{I}_{(\mathfrak{t}_1,0)}(X_kT_1)))(\tau) = -i\tau\frac{1}{8}\mathscr{C}_\Delta(k)\varphi_1\left(2i\tau\frac{1}{\varepsilon^2}\right)e^{i\tau\left(\frac{1}{\varepsilon^2}+\mathscr{B}_\Delta(k)\right)}.$$

Together with the observation that

$$\frac{\Upsilon^p(X_kT_1)(v)}{S(T_1)} = \hat{v}_{k_1}\hat{v}_{k_2}\hat{v}_{k_3}$$

we obtain for the first tree T_1 in Fourier space that

$$\begin{aligned}\frac{\Upsilon^p(X_kT)(v)}{S(T)}&\Pi_n(\mathscr{D}_0(\mathscr{I}_{(\mathfrak{t}_1,0)}(X_kT_1)))(\tau)\\ &= -i\tau\frac{1}{8}\mathscr{C}_\Delta(k)\hat{v}_{k_1}\hat{v}_{k_2}\hat{v}_{k_3}\varphi_1\left(2i\tau\frac{1}{\varepsilon^2}\right)e^{i\tau\left(\frac{1}{\varepsilon^2}+\mathscr{B}_\Delta(k)\right)}.\end{aligned}$$

In physical space the latter takes the form

$$\begin{aligned}\mathscr{F}^{-1}&\left(\frac{\Upsilon^p(X_kT)(v)}{S(T)}\Pi_n(\mathscr{D}_0(\mathscr{I}_{(\mathfrak{t}_1,0)}(X_kT_1)))(\tau)\right)\\ &= -i\frac{1}{8}\tau e^{i\tau\left(\frac{1}{\varepsilon^2}+\mathscr{B}_\Delta\right)}\mathscr{C}_\Delta\varphi_1\left(2i\tau\frac{1}{\varepsilon^2}\right)v^3\end{aligned} \tag{A.45}$$

with $\mathscr{B}_\Delta$ and $\mathscr{C}_\Delta$ defined in (A.38). The term (A.45) is exactly the third term (corresponding to $(u^\ell)^3$) in the first-order scheme (A.40). The other terms in the scheme can be computed in a similar way with the aid of the trees T_j, $j = 1, 2, 3, 4$. The local error is then given by Theorem 4.7. For instance, the local error introduced by the approximation of T_1 reads

$$\mathcal{O}\left(\tau^2(-\mathscr{B}_\Delta(k) + \mathscr{B}_\Delta(k_1) + \mathscr{B}_\Delta(k_2) + \mathscr{B}_\Delta(k_3))\hat{v}_{k_1}\hat{v}_{k_2}\hat{v}_{k_3}\right) = \mathcal{O}(\tau^2\Delta v^3).$$

The other approximations obey a similar error structure.

The simplified scheme (A.41) on the other hand is constructed by carrying out a Taylor series expansion of the full operator $\mathscr{L}_{\text{dom}} + \mathscr{L}_{\text{low}}$. For instance, when calculating $\mathscr{K}$, instead of integrating the dominant part (A.44) for the first tree T_1, exactly, we Taylor expand the full operator

$$P_{(\mathfrak{t}_2,0)}\left(k, \frac{1}{\varepsilon^2}\right) + P = 2\frac{1}{\varepsilon^2} - \mathscr{B}_\Delta(k) + \mathscr{B}_\Delta(k_1) + \mathscr{B}_\Delta(k_2) + \mathscr{B}_\Delta(k_3).$$

This implies a local error structure of type

$$\mathcal{O}\left(\frac{\tau^2}{\varepsilon^2}u\right) + \mathcal{O}(\tau^2\Delta u)$$

We omit further details here.

□

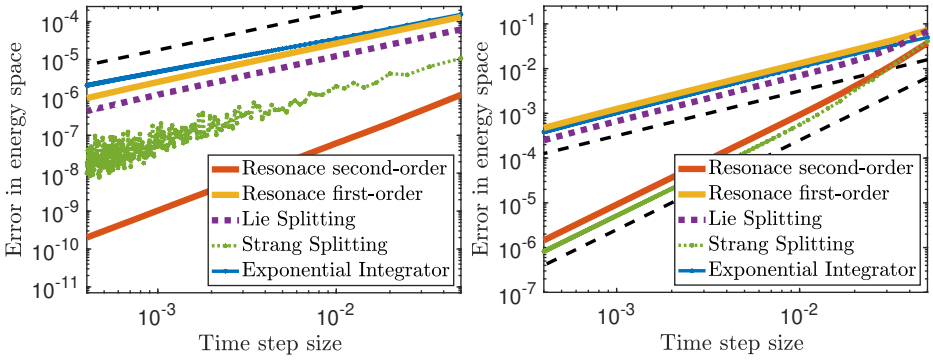
Remark A.9 Our framework (4.12) allows us to also derive second- and higher-order schemes for the Klein–Gordon equation (A.37). The trees have the same shape as for the cubic Schrödinger equation (A.1), but many more trees $T \in \mathcal{T}_0^3(R)$ are needed for the description. With our framework we can in particular recover the first- and second-order uniformly accurate method proposed in [5].

A.4 Numerical experiments

We underline the favorable error behavior of the new resonance based schemes compared to classical approximation techniques in case of non-smooth solutions. We choose $M = 2^8$ spatial grid points and carry out the simulations up to $T = 0.1$.

Example 7 (Schrödinger) In Figure 3 we compare the convergence of the new resonance based approach with classical splitting and exponential integration schemes in case of the Schrödinger equation (A.1) with smooth and non-smooth solutions. The numerical experiments underline the favorable error behavior of the resonance based schemes presented in Corollary A.3 in case of non-smooth solutions. While the second-order Strang splitting faces high oscillations in the error causing severe order reduction, the second-order resonance based scheme maintains its second-order convergence for less regular solutions.

Example 8 (Kortweg–de Vries) Figure 4 underlines the preferable choice of embedding the resonance structure into the numerical discretisation even for smooth solutions of the KdV equation (A.30). While the second-order classical exponential integrator suffers from spikes in the error when hitting certain (resonant) time steps, the second-order resonance based scheme presented in Corollary A.5 allows for full-order convergence without any oscillations.



(a) H^2 data (b) $\mathscr{C}^\infty$ data

Figure 3: Error versus step size (double logarithmic plot). Comparison of classical and resonance based schemes for the Schrödinger equation for smooth (right picture) and non-smooth (left picture) solutions.

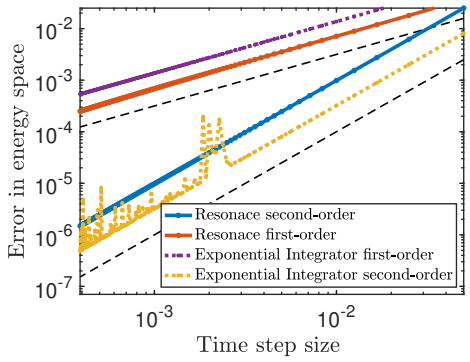


Figure 4: Error versus step size (double logarithmic plot). Comparison of classical and resonance based schemes for the KdV equation with smooth data in $\mathscr{C}^\infty$.

References

[1] W. Bao, X. Zhao, *A uniformly accurate multiscale time integrator spectral method for the Klein-Gordon-Zakharov system in the high-plasma-frequency limit regime*, J. Comput. Phys 327:270–293 (2016)

[2] W. Bao, Y. Cai, X. Zhao, *A uniformly accurate multiscale time integrator pseudospectral method for the Klein-Gordon equation in the nonrelativistic limit regime*, SIAM J. Numer. Anal. 52:2488-2511 (2014)

[3] W. Bao, X. Dong, *Analysis and comparison of numerical methods for the Klein-Gordon equation in the nonrelativistic limit regime*, Numer. Math. 120:189–229 (2012)

[4] S. Baumstark, K. Schratz, *Uniformly accurate oscillatory integrators for the Klein–Gordon–Zakharov system from low- to high-plasma frequency regimes.* SIAM J. Numer. Anal. 57:429–457 (2019)

[5] S. Baumstark, E. Faou, K. Schratz, *Uniformly accurate oscillatory integrators for Klein–Gordon equations with asymptotic convergence to the classical NLS splitting.*

Math. Comp. 87:1227–1254 (2018)

[6] N. Berglund, Y. Bruned. *BPHZ renormalisation and vanishing subcriticality limit of the fractional φ^3_d model.* arXiv:1907.13028.

[7] H. Berland, B. Owren, B. Skaflestad, *B-series and order conditions for exponential integrators.* SIAM J. Numer. Anal., 43: 1715–1727 (2015)

[8] C. Besse, B. Bidégaray, S. Descombes, *Order estimates in time of splitting methods for the nonlinear Schrödinger equation.* SIAM J. Numer. Anal. 40:26–40 (2002).

[9] J. Bourgain, *Fourier transform restriction phenomena for certain lattice subsets and applications to nonlinear evolution equations. Part I: Schrödinger equations.* Geom. Funct. Anal. 3:209–262 (1993).

[10] Y. Bruned. *Recursive formulae in regularity structures.* Stoch. Partial Differ. Equ. Anal. and Comput. **6**, no. 4, (2018), 525–564. doi:10.1007/s40072-018-0115-z.

[11] Y. Bruned, A. Chandra, I. Chevyrev, M. Hairer. *Renormalising SPDEs in regularity structures*. to appear in J. Eur. Math. Soc. arXiv:1711.10239.

[12] Y. Bruned, M. Hairer, L. Zambotti. *Algebraic renormalisation of regularity structures.* Invent. Math. **215**, no. 3, (2019), 1039–1156. doi:10.1007/s00222-018-0841-x.

[13] Y. Bruned, M. Hairer, L. Zambotti. *Renormalisation of Stochastic Partial Differential Equations.* EMS Newsletter **115**, no. 3, (2020), 7–11. doi:10.4171/NEWS/115/3.

[14] Y. Bruned, F. Gabriel, M. Hairer, L. Zambotti. *Geometric stochastic heat equations*. arXiv:1902.02884.

[15] N. Burq, P. Gérard, N. Tzvetkov. *Strichartz inequalities and the nonlinear Schrödinger equation on compact manifolds.* Amer. J. Math. 126:569–605 (2004).

[16] J. C. Butcher. *An algebraic theory of integration methods.* Math. Comp. **26**, (1972), 79–106. doi:10.2307/2004720.

[17] J. Butcher. *Numerical Methods for Ordinary Differential Equations.* third edition, 2016, Wiley

[18] J. Butcher *Trees, B-series and exponential integrators.* IMAJNA **30**:131–140 (2010)

[19] D. Calaque, K. Ebrahimi-Fard, D. Manchon. *Two interacting Hopf algebras of trees: a Hopf-algebraic approach to composition and substitution of B-series.* Adv. in Appl. Math. **47**, no. 2, (2011), 282–308. doi:10.1016/j.aam.2009.08.003.

[20] B. Cano, A. González-Pachón, *Exponential time integration of solitary waves of cubic Schrödinger equation.* Appl. Numer. Math. 91:26–45 (2015)

[21] E. Celledoni, D. Cohen, B. Owren, *Symmetric exponential integrators with an application to the cubic Schrödinger equation.* Found. Comput. Math. 8:303–317 (2008).

[22] A. Chandra, M. Hairer. *An analytic BPHZ theorem for Regularity Structures.* arXiv:1612.08138v5.

[23] A. Chandra, M. Hairer, H. Shen. *The dynamical sine-Gordon model in the full subcritical regime.* arXiv:1808.02594.

[24] A. Chandra, A. Moinat, H. Weber. *A priori bounds for the φ^4 equation in the full sub-critical regime.* arXiv:1910.13854.

[25] P. Chartier, N. Crouseilles, M. Lemou, F. Méhats, *Uniformly accurate numerical schemes for highly oscillatory Klein-Gordon and nonlinear Schrödingier equations*, Numer. Math. 129:211-250 (2015)

[26] P. Chartier, E. Hairer, G. Vilmart. *Algebraic structures of B-series.* Found. Comput. Math. **10**, no. 4, (2010), 407–427. doi:10.1007/s10208-010-9065-1.

[27] M. Christ, *Power series solution of a nonlinear Schrödinger equation.* In Mathematical aspects of nonlinear dispersive equations, volume 163 of Ann. of Math. Stud., pages 131–155. Princeton Univ. Press, Princeton, NJ, 2007

[28] D. Cohen, E. Hairer, C. Lubich, *Modulated Fourier expansions of highly oscillatory differential equations*, Foundations of Comput. Math. 3:327–345 (2003)

[29] D. Cohen, L. Gauckler, *One-stage exponential integrators for nonlinear Schrödinger equations over long times.* BIT 52:877–903 (2012).

[30] A. Connes, D. Kreimer. *Hopf algebras, renormalization and noncommutative geometry.* Comm. Math. Phys. **199**, no. 1, (1998), 203–242. doi:10.1007/s002200050499.

[31] A. Connes, D. Kreimer. *Renormalization in quantum field theory and the Riemann-Hilbert problem I: the Hopf algebra structure of graphs and the main theorem.* Commun. Math. Phys. **210**, (2000), 249–73. doi:10.1007/s002200050779.

[32] R. Coifman, Y. Meyer, *On commutators of singular integrals and bilinear singular integrals*. Trans. Amer. Math. Soc. 212:315-331 (1975)

[33] G. Dujardin, *Exponential Runge–Kutta methods for the Schrödinger equation.* Appl. Numer. Math. 59:1839–1857 (2009).

[34] B. Engquist, A. Fokas, E. Hairer, A. Iserles, *Highly Oscillatory Problems.* Cambridge University Press, 2009

[35] E. Faou, Geometric Numerical Integration and Schrödinger Equations. European Math. Soc. Publishing House, Zürich, 2012.

[36] B. Fornberg, *Generation of Finite Difference Formulas on Arbitrarily Spaced Grids*, Math. Comp. 51:699–706 (1988)

[37] L. Gauckler, C. Lubich, *Nonlinear Schrödinger equations and their spectral semi-discretisations over long times.* Found. Comput. Math. 20:141–169 (2010).

[38] Z. Guo, S. Kwon, T. Oh, *Poincaré-Dulac normal form reduction for unconditional well-posedness of the periodic cubic NLS*, Comm. Math. Phys. 322 (2013), no. 1, 19–48.

[39] M. Gubinelli. *Controlling rough paths.* J. Funct. Anal. **216**, no. 1, (2004), 86–140.

[40] M. Gubinelli. *Ramification of rough paths.* J. Differ. Equ. **248**, no. 4, (2010), 693 – 721. doi:10.1016/j.jde.2009.11.015.

[41] M. Gubinelli, *Rough solutions for the periodic Korteweg-de Vries equation.* Comm. Pure Appl. Anal. 11:709–733 (2012).

[42] E. Hairer, S. Nørsett, G. Wanner, *Solving Ordinary Differential Equations I: Nonstiff problems*Springer, Berlin, 1987

[43] E. Hairer, C. Lubich, G. Wanner, *Geometric numerical integration. Structure-preserving algorithms for ordinary differential equations.* second ed., vol. 31 of Springer Series in Computational Mathematics, Springer-Verlag, Berlin, 2006.

[44] M. Hairer. *A theory of regularity structures.* Invent. Math. **198**, no. 2, (2014), 269–504. doi:10.1007/s00222-014-0505-4.

[45] M. Hairer, P. Schönbauer. *The support of singular stochastic PDEs.* arXiv:1909.05526.

[46] M. Hochbruck, A. Ostermann, *Exponential integrators.* Acta Numer. 19:209–286 (2010).

[47] M. Hofmanová, K. Schratz, *An oscillatory integrator for the KdV equation*, Numer. Math. 136:1117-1137 (2017).

[48] H. Holden, K. H. Karlsen, K.-A. Lie, N. H. Risebro, *Splitting for Partial Differential Equations with Rough Solutions.* European Math. Soc. Publishing House, Zürich (2010).

[49] H. Holden, C. Lubich, N. H. Risebro, *Operator splitting for partial differential equations with Burgers nonlinearity.* Math. Comp. 82:173–185 (2012).

[50] H. Holden, K. H. Karlsen, N. H. Risebro, T. Tao, *Operator splitting methods for the Korteweg-de Vries equation.* Math. Comp. 80:821–846 (2011).

[51] H. Holden, K. H. Karlsen, N. H. Risebro, *Operator splitting methods for generalized Korteweg-de Vries equations*. J. Comput. Phys. 153:203–222 (1999).

[52] L. Ignat, E. Zuazua, *Numerical dispersive schemes for the nonlinear Schrödinger equation*. SIAM J. Numer. Anal. 47:1366–1390 (2009).

[53] A. Iserles, G.R.W. Quispel, P.S.P. Tse, B-series methods cannot be volume-preserving. BIT Numerical Mathematics 47:351–378 (2007)

[54] T. Jahnke, C. Lubich, *Error bounds for exponential operator splittings.* BIT, 40:735–744 (2000).

[55] C. Klein, *Fourth order time-stepping for low dispersion Korteweg-de Vries and nonlinear Schrödinger equation.* ETNA 29:116–135 (2008).

[56] M. Keel, T. Tao. *Endpoint Strichartz estimates.* Amer. J. Math. 120:955–980 (1998).

[57] M. Knöller, A. Ostermann, K. Schratz, *A Fourier integrator for the cubic nonlinear Schrödinger equation with rough initial data.* SIAM J. Numer. Anal. 57:1967-1986 (2019) .

[58] C. Lubich, *On splitting methods for Schrödinger-Poisson and cubic nonlinear Schrödinger equations.* Math. Comp. 77:2141–2153 (2008).

[59] B. Leimkuhler, S. Reich, *Simulating Hamiltonian dynamics.* Cambridge Monographs on Applied and Computational Mathematics 14. Cambridge University Press, Cambridge, 2004

[60] T. Lyons. *On the nonexistence of path integrals.* Proc. Roy. Soc. London Ser. A **432**, no. 1885, (1991), 281–290.

[61] T. J. Lyons. *Differential equations driven by rough signals.* Rev. Mat. Iberoamericana **14**, no. 2, (1998), 215–310.

[62] Y. Maday, A. Quarteroni, *Error analysis for spectral approximation of the Korteweg-de Vries equation.* RAIRO - Modélisation mathématique et analyse numérique 22:821–846 (1988).

[63] R.I. McLachlan, G.R.W. Quispel, *splitting methods.* Acta Numer. 11:341–434 (2002)

[64] H. Munthe-Kaas, K. Føllesdal, *Lie-Butcher series, geometry, algebra and computation.* Springer Lectues in Mathematics and Statistics, 2017.

[65] A. Murua, J.M. Sanz-Serna, *Word Series for Dynamical Systems and Their Numerical Integrators.* Found. Comp. Math 17:675–712 (2017)

[66] A. Ostermann, C. Su, *Two exponential-type integrators for the "good" Boussinesq equation.* Numer. Math. 143:683–712 (2019)

[67] A. Ostermann, K. Schratz, *Low regularity exponential-type integrators for semilinear Schrödinger equations*, Found. Comput. Math. 18:731–755 (2018).

[68] A. Ostermann, F. Rousset, K. Schratz, *Error estimates of a Fourier integrator for the cubic Schrödinger equation at low regularity* (to appear in Found. Comput. Math.) arXiv:1902.06779.

[69] J.M. Sanz-Serna, M.P. Calvo, *Numerical Hamiltonian Problems.* Chapman and Hall, London, 1994

[70] K. Schratz, Y. Wang, X. Zhao, *Low-regularity integrators for nonlinear Dirac equations.* (to appear in Math. Comput.) arxiv:1906.09413

[71] R. S. Strichartz. *Restrictions of Fourier transforms to quadratic surfaces and decay of solutions of wave equations.* Duke Math. J. 44:705–714 (1977).

[72] T. Tao, Nonlinear Dispersive Equations. Local and Global Analysis. Amer. Math. Soc., Providence RI, 2006.

[73] F. Tappert, *Numerical solutions of the Korteweg-de Vries equation and its generalizations by the split-step Fourier method.* In: (A. C. Newell, editor) Nonlinear Wave Motion, Amer. Math. Soc. 215–216 (1974).

[74] M. Thalhammer, *Convergence analysis of high-order time-splitting pseudo-spectral methods for nonlinear Schrödinger equations.* SIAM J. Numer. Anal. 50:3231–3258 (2012).